

#### IV. THE ROLE OF AROMATIC HYDROCARBONS IN POLLUTED URBAN ATMOSPHERES: DEVELOPMENT AND VALIDATION OF MECHANISMS OF PHOTOOXIDATION

Aromatic hydrocarbons are recognized to be an important constituent of anthropogenic emissions in polluted urban atmospheres (Lonneman et al., 1974). In order to develop chemical kinetic computer models of photochemical air pollution as an integral part of urban airshed models for the formulation of emission control strategies, the chemistry involved in the photooxidation of these aromatic hydrocarbons under atmospheric conditions must be reasonably well understood (Finlayson-Pitts and Pitts, 1977). As a first step, such computer kinetic models must, as far as possible, be validated against accurate smog chamber data, even though it is recognized that there are significant wall effects associated with smog chambers (Carter et al., 1979). At the present time, while reasonably validated detailed chemical kinetic computer models exist for the n-butane (a representative short chain [ $\leq C_4$ ] alkane) and propene (a representative alkene)- $NO_x$ -air systems (Carter et al., 1979; Hendry et al., 1978), the chemistry occurring in the  $NO_x$  photooxidations of the aromatic hydrocarbons is still incompletely understood (Atkinson et al., 1979).

In recent years laboratory studies have shown that under atmospheric conditions the major initial reaction of the aromatics is with the hydroxyl radical and data are now available concerning both the overall OH radical rate constants (Atkinson et al., 1979, and references contained therein; Hendry, 1979) and the relative amounts of OH radical addition and H atom abstraction (Atkinson et al., 1979; Hendry, 1979) for many of these compounds. Additionally, the reactions of ozone with the aromatic hydrocarbons, leading to the production of  $\alpha$ -dicarbonyls have been shown to be negligible under atmospheric conditions (Pate et al., 1976a; Bufalini and Altshuller, 1965; Stedman and Niki, 1973).

Several product studies of irradiated  $NO_x$ -aromatic-air systems (mainly of the  $NO_x$ -toluene-air system) have been carried out (Altshuller et al., 1970; Spicer and Jones, 1977; Grosjean et al., 1978; Akimoto et al., 1978; O'Brien et al., 1979; Pitts et al., 1979b). Quantitative measurements of a large variety of products and of the reactants under carefully controlled experimental conditions have not been available.

Products which retain the aromatic ring have been observed, including benzaldehyde, benzyl nitrate, cresols, nitrotoluene and nitrocresols in the gas phase (Altshuller et al., 1970; Spicer and Jones, 1977; Grosjean et al., 1978; Akimoto et al., 1978; O'Brien et al., 1979; Pitts et al., 1979b) and dihydroxynitrotoluenes in the aerosol phase (Grosjean et al., 1978). The formation of large yields of products such as PAN, CO, and HCHO in the toluene- $\text{NO}_x$  irradiations (Grosjean et al., 1978; O'Brien et al., 1979; Pitts et al., 1979b) and the recent observation of significant yields ( $18 \pm 4\%$  of the total reaction) of biacetyl in irradiated  $\text{NO}_x$ -o-xylene-air mixtures (Darnall et al., 1979) indicate the importance of ring cleavage.

Recently Hendry and co-workers (1978) have formulated a detailed chemical computer model for the  $\text{NO}_x$  photooxidation of toluene involving aromatic ring cleavage only after cresol formation, i.e., OH radical addition to toluene yields mainly o-cresol, with the o-cresol reacting further with OH radical to yield a variety of ring cleavage products. However, it has been shown (Darnall et al., 1979) that the rate determining step for the formation of the ring cleavage product biacetyl from the reaction of OH radicals with o-xylene was that for the initial reaction of OH radicals with o-xylene, and that its production from the reaction of OH radicals (or ozone) with a hydroxyxylene would have led to an incorrect biacetyl concentration-time profile.

In this section product studies of toluene- $\text{NO}_x$ -air, toluene-benz-aldehyde- $\text{NO}_x$ -air, and cresol- $\text{NO}_x$ -air mixtures irradiated under controlled conditions in an environmental chamber are presented, and a reaction scheme which employs the available kinetic and mechanistic information and is based in part upon a previously-developed chemical computer model for the n-butane-propene- $\text{NO}_x$ -air system (Carter et al., 1979) is formulated. Some of the detailed chemistry is, by necessity, speculative, but this reaction scheme fits the data reasonably well over a significant range of initial reactant levels.

Experimental. The apparatus and general techniques used have been described previously (Pitts et al., 1979b; Pitts, et al., 1977; Darnall et al., 1979). Irradiations were carried out in the 5800-liter evacuable, Teflon-lined, thermostatted environmental chamber (Winer et al., 1980)

using a 25 KW solar simulator. Prior to each run the chamber was evacuated to pressures of  $\sim 10^{-5}$  torr, and was then filled with purified matrix air (Doyle et al., 1977) humidified to  $\sim 50\%$  relative humidity (RH) at  $303 \pm 1$  K. Toluene or the cresols, and NO and  $\text{NO}_2$  were injected into the chamber using precision bore syringes, while benzaldehyde was expanded into the evacuated chamber from known benzaldehyde- $\text{N}_2$ -mixtures prepared in a 5.5-liter bulb. All reactants were allowed to mix for at least 30 minutes before  $t = 0$ . During a run the temperature of the irradiated mixture was maintained at the desired value by means of the chamber refrigeration or heating system.

The parameters monitored and the methods employed were:  $\text{O}_3$  by UV absorbance (Dasibi Model 1212); NO,  $\text{NO}_2$ , and  $\text{NO}_x$  by chemiluminescence (Winer et al., 1974;  $\text{NO}_2$  and  $\text{NO}_x$  values are corrected for response to PAN and alkyl nitrates) (Thermo Electron Model 14B); CO by gas chromatography (Beckman 6800); RH by a thin film, bulk effect humidity sensor (Brady Array); light intensity and spectral distribution by a photodiode and an absolute radiometer (EG&G), and by a double monochromator-photo-multiplier combination, respectively (Pitts et al., 1979b); and HCHO using an improved chromotropic acid method (Pitts et al., 1979b; Darnall et al., 1979; Smith et al., 1970). The absolute light intensity was determined periodically using the rate of photolysis of  $\text{NO}_2$  in  $\text{N}_2$  to determine  $k_1$  (Holmes et al., 1973).

Benzaldehyde, benzyl nitrate, cresols, nitrotoluenes, and hydroxy-nitrotoluenes were monitored by gas chromatography (GC) with flame ionization detection (FID) (Pitts et al., 1979b) using either (a) a  $10' \times 1/4"$  (2mm i.d.) borosilicate glass column packed with 60/80 mesh Tenax GC, temperature programmed from 373 to 523 K at 20 K per minute, or (b) a  $6' \times 1/4"$  0.1% SP 1000/Carbopack C (Supelco) column, temperature programmed from 423 K to 523 K at 20 K per minute. In both cases 10.8- or 3.6-liter gas samples from the chamber were drawn through a  $1/4" \times 3 1/4"$  borosilicate glass trap packed with 1 1/2" Tenax GC 60/80 mesh. The sample was then transferred by the carrier gas at 528 K from this trap to the column head which was at 373 or 423 K, followed by the temperature programming of the columns as noted above.

Peroxyacetyl nitrate (PAN) and methyl nitrate were monitored by GC using an 18" x 1/8" Teflon column of 5% Carbowax 400 on Chromosorb G (80/100 mesh) operated at 301 K with electron capture detection (ECD) (Darley et al., 1963; Stephens and Price, 1973). Toluene and the oxy- genates were monitored employing a 10' x 1/8" stainless steel (SS) column of 10% Carbowax 600 on C-22 firebrick (100/20 mesh) (Pitts et al., 1979b; Darnall et al., 1979; Stephens, 1973). In later runs, toluene and benz- aldehyde were monitored employing a 5' x 1/8" SS column of 5% Carbowax 600 on C-22 firebrick (100/115 mesh) for which the sampling trap and injection valve was heated to 368-373 K (Pitts et al., 1979b). Acetylene and back- ground alkanes and alkenes were monitored on Porapak N or 2,4-dimethyl- sulfolane columns as described previously (Pitts et al., 1979b; Darnall et al., 1979; Stephens, 1973).

The reliability of the reactant and product analyses employing these techniques is estimated (Pitts et al., 1979b; Darnall et al., 1979) to be as follows: O<sub>3</sub> and NO,  $\pm 5\%$ ; NO<sub>2</sub>, at best  $\pm 5\%$  but more uncertain due to uncertainties in the measurements of interfering compounds (Winer et al., 1974) and the possibility of interferences from unmonitored compounds; CO,  $\pm 10\%$ ; toluene,  $\pm 10\%$ ; aromatic products monitored on the SP-1000 or the Tenax GC system, at best  $\pm 25\%$ ; benzaldehyde on the 5' Carbowax 600 system,  $\pm 10\%$ ; PAN  $\pm 20\%$ ; formaldehyde, +10 to -30%; and methyl nitrate,  $\pm 50\%$ .

In addition, qualitative analyses of the aromatic products (benzal- dehyde, benzyl nitrate, cresols, nitrotoluenes, and hydroxynitrotoluenes) were carried out using a Finnigan 3100-combined gas chromatograph-mass spectrometer (GC-MS), with a 6100 data system (Glangetas, 1978). A 26- meter x 0.29-mm i.d. glass capillary column coated with Ucon-50-HB-5100 polypropylene glycol, temperature programmed from 313 K to 492 K at 8 K min<sup>-1</sup> was employed for these analyses.

Product assignments were made by comparison of the retention times (FID and ECD) and/or mass spectra (GC-MS) (Glangetas, 1978) with authentic samples, wherever possible.

Most calculations were carried out at Riverside as discussed previous- ly (Carter et al., 1979). Input parameters consisted of the initial concentrations of the reactants, a reaction mechanism consisting of a list

of reactions and their rate constants, or photolysis rates, which is given in Appendix A together with the relevant notes and references, and the dilution rate. The set of differential equations resulting from this reaction mechanism were integrated using the Gear algorithm (Gear, 1971; Hindmarsh, 1972). Initial exploratory calculations were carried out on a Univac 1108 computer at Shell Research Ltd., Thornton Research Centre, Chester, UK, using an implicit one-step method with single precision to solve stiff ordinary differential equations (Prothero and Robinson, 1974).

The reaction scheme used in our model calculations, along with associated references and notes, is given in Appendix A. The inorganic reactions (reactions 1-34) are essentially identical to those used recently by Carter et al. (1979) for the  $\text{NO}_x$ -n-butane-propene-air system, apart from a minor updating of rate constants. Hence, the inorganic reaction scheme will not be discussed in any detail here; Appendix A should be consulted for further details. Analogous to this previous (Carter et al., 1979) and the other recent (Hendry et al., 1978) modeling studies, a constant (for a given run) chamber radical source was found necessary in order to match the calculated and the experimental time-concentration profiles; and as before (Carter et al., 1979), these radicals were presumed to be OH radicals (see note 8 of Appendix A).

The organic reaction scheme is given in Appendix A as reactions 35-166; reactions 46-53 and 70-77 represent overall processes whose detailed reactions are given for aromatic systems in general in Appendix B. The general reactions listed in Appendix B were applied to both the toluene- $\text{NO}_x$ -air and the o-cresol- $\text{NO}_x$ -air mechanisms, and are intended to be applicable to the  $\text{NO}_x$ -air photooxidations of all substituted benzenes (see notes 14-19, 26 and 27 of Appendix A and the discussion below). A number of possible alternative mechanisms, discussed below, were examined, and the appendices list all reactions considered, including those which were subsequently found to give unacceptable fits to the data. Throughout the discussion, unprimed reaction numbers (e.g., 35, 36, etc.) will refer to those in Appendix A, while primed reaction numbers (e.g., 1', 2', etc.) will refer to specific examples of the general reactions in Appendix B.

Experimental Results. Initial conditions and selected reactivity

parameters for the experiments reported here are given in Table 11. In order to check reproducibility several duplicate irradiations were carried out. In those cases, very similar reactivity parameters were observed (especially for runs carried out with the same solar simulator lamp [Pitts et al., 1979b; Darnall et al., 1979], which was changed between runs 290 and 327), and product yields agreed to within their stated uncertainty limits (compare runs 264-266 and 327 and 340).

The products observed in the toluene- $\text{NO}_x$ -air runs for which quantitative results were obtained (in approximate order of yield) were CO, formaldehyde, PAN, benzaldehyde, o-cresol, m-nitrotoluene, acetylene, and methyl nitrate. Also detected (Glangetas, 1978) were small amounts of m- and p-cresol, o- and p-nitrotoluene, benzyl nitrate, and 2,3-, 2,5-, 3,2-, 3,4-, and 4,3-hydroxynitrotoluenes. In the cresol- $\text{NO}_x$ -air runs, the products detected were CO, PAN, and 2,3- and 2,5-hydroxynitrotoluenes from o-cresol; CO, PAN and 3,2- and 3,4-hydroxynitrotoluenes from m-cresol, and CO, PAN and 4,3-hydroxynitrotoluene from p-cresol. The organic product yields in the cresol runs were very low and the PAN yields were much lower than those observed in the toluene runs. The maximum yields of the major organic products observed in the toluene- $\text{NO}_x$ -air and toluene-benzaldehyde- $\text{NO}_x$ -air irradiations are given in Table 12.

Figure 36 compares the concentration-time profiles observed for  $\text{O}_3$ , NO,  $\text{NO}_2$ , PAN and the reactant cresol in the o-, m-, and p-cresol- $\text{NO}_x$ -air runs. (The nonzero initial ozone values observed are believed to be due to a cresol interference on the UV absorbance  $\text{O}_3$  monitor.) In addition, concentration-time profiles for selected species observed in the o-cresol and in selected toluene and toluene-benzaldehyde runs are plotted in Figures 37 - 42, along with results of model calculations (discussed below). In general, it can be seen that the cresol runs and the added benzaldehyde runs have a lower overall reactivity than comparable toluene runs, and that m-cresol is by far the most reactive of the cresol isomers. These results can be rationalized in terms of the mechanism which is discussed below.

Detailed data tabulations, giving concentrations of all organic and inorganic species monitored, and values of measured physical parameters as a function of time, including the spectral distribution of the photolysis-

Table 11

Initial conditions and selected reactivity parameters for the irradiated toluene- $\text{NO}_x$ -air, toluene-benzaldehyde- $\text{NO}_x$ -air and cresol- $\text{NO}_x$ -air mixtures

Run	EC-264	EC-265	EC-266	EC-269	EC-271	EC-273	EC-281	EC-289	EC-290	EC-327	EC-337	EC-339	EC-340
<u>Reactants (ppm)</u>													
Toluene	1.156	1.070	1.196	0.566	1.146	0.587	0.394	0.297		0.573	0.959	0.536	0.537
o-Cresol													
m-Cresol													
p-Cresol													
Benzaldehyde													
NO	0.420	0.435	0.432	0.398	0.186	0.096	0.458	0.404	0.413	0.357	0.172	0.187	
$\text{NO}_2$	0.056	0.048	0.059	0.074	0.029	0.014	0.020	0.045	0.067	0.096	0.124	0.102	0.096
$\text{NO}_x$	0.470	0.482	0.494	0.472	0.215	0.110	0.480	0.449	0.481	0.448	0.448	0.445	0.430
<u>Physical Parameters</u>													
$k_1$ ( $\text{min}^{-1}$ )	0.35	0.35	0.35	0.37	0.37	0.35	0.39	0.39	0.40	0.39	0.39	0.39	0.39
Ave. Temp. (K)	304.5	302.6	302.8	302.9	303.0	303.6	302.9	303.0	303.1	303.4	303.0	303.4	303.1
Ave. RH (%)	42.0	54.0	47.5	46.5	49.5	49.5	48.0	56.5	52.4	~60	65.6	64.0	63.2
<u>Reactivity Parameters</u>													
Max. $\text{O}_3$ (ppm)	0.419	0.393	0.403	>0.298*	0.296	0.215	>0.064*	0.137	>0.068*	0.376	0.325	>0.225*	0.346
Time $\text{O}_3$ max. (min.)	210	210	215	>360	90	80	>360	210	>360	~360	255	>360	360

\* 6-hour value given.

Table 12

Observed and Calculated<sup>a</sup> Maximum Product Yields in the Toluene and Toluene-Benzaldehyde-NO<sub>x</sub>-Air Runs

Run		EC-266 <sup>b</sup>	EC-269	EC-271	EC-273	EC-337	EC-339	EC-340 <sup>b</sup>
Products (ppb)	Obs.	Calc.	Obs.	Calc.	Obs.	Calc.	Obs.	Calc.
<u>Aromatic</u>								
Benzaldehyde	22 <sup>c</sup>	23	9 <sup>d</sup>	12	17 <sup>d</sup>	18	16 <sup>d</sup>	10
o-Cresol	9 <sup>c</sup>	18	7	10	13	14	11	12
m-Cresol	2 <sup>c</sup>	NC <sup>f</sup>	1 <sup>c</sup>	NC	--	NC	--	NC
p-Cresol	2 <sup>c</sup>	NC	0.7 <sup>c</sup>	NC	--	NC	--	NC
o-Nitrotoluene	0 <sup>c</sup>	NC	1 <sup>c</sup>	NC	0.1	NC	0.6	NC
m-Nitrotoluene	3 <sup>c</sup>	0.2	1 <sup>c</sup>	0.1	--	<0.1	0.3	0.3
p-Nitrotoluene	4 <sup>c</sup>	NC	0.9 <sup>c</sup>	NC	--	NC	0.3	NC
$\Sigma$ Hydroxynitrotoluenes	--	NC	6.7 <sup>c</sup>	NC	--	NC	--	NC
Benzyl nitrate <sup>g</sup>	--	14	0.8 <sup>c</sup>	10	--	8	--	4
PBzN	--	9	--	9	--	3	--	2
Other Organic Nitrates <sup>g,h</sup>	--	60	--	48	--	35	--	21
<u>Fragmentation</u>								
PAN	75	91	50	52	60	31	32	47
Other peroxy nitrates <sup>i</sup>	--	67	--	56	--	29	--	17
Glyoxyl	--	18	--	19	--	7	--	5
Methyl glyoxyl	--	21	--	10	--	21	--	12
2-Butene-1,4-dial	--	75	--	39	--	64	--	36
Formaldehyde	75	31	40	26	42	17	17	11
Methyl nitrate <sup>g</sup>	1	0.6	1	0.6	--	0.1	<0.1	0.6
CO <sup>j</sup>	500	202	~300	211	(e)	(e)	(e)	(e)
Acetylene <sup>j</sup>	--	NC	--	NC	--	NC	2.4	NC

Table 12 (continued)

<u>Notes</u>
<sup>a</sup> Calculated using model A. Yields given are maximum calculated at the time of complete NO <sub>2</sub> consumption, or at 6 hours, whichever came first.
<sup>b</sup> Duplicate runs done gave either less well characterized product data, or data which was consistent with results given here.
<sup>c</sup> Only semi-quantitative GC/MS data [47] is available.
<sup>d</sup> Chromatographic column employed could not separate benzaldehyde and benzyl nitrate, so reported data is benzaldehyde + benzyl nitrate.
<sup>e</sup> Present as a reactant in this run.
<sup>f</sup> NC = Not calculated. Assumed to be negligible in the model.
<sup>g</sup> Reactions consuming this product were not included in the model, so the actual calculated yields should be smaller.
<sup>h</sup> Primarily C <sub>7</sub> ONO <sub>2</sub> formed in Reactions 46-53.
<sup>i</sup> Primarily HCOCH=CHCO <sub>3</sub> NO <sub>2</sub> formed in Reaction 112.
<sup>j</sup> Background levels subtracted.

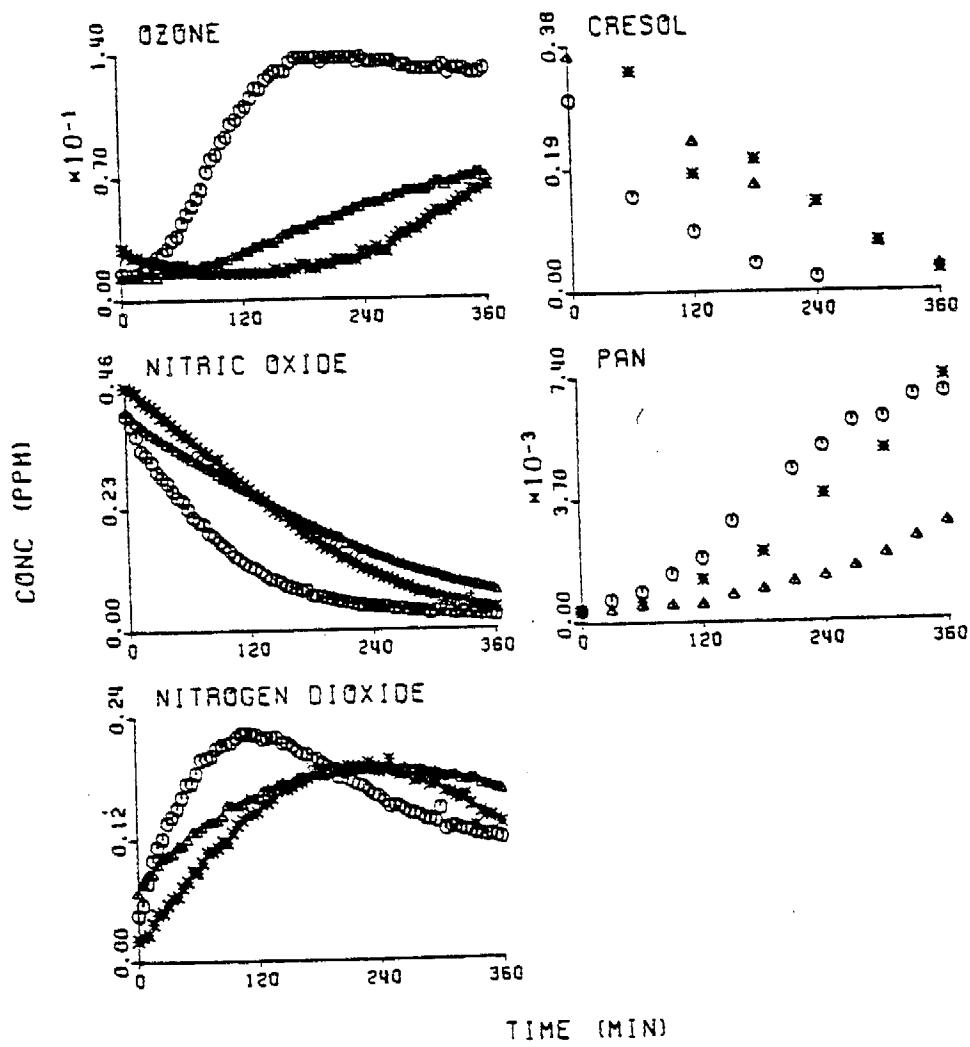


Figure 36. Concentration-Time Profiles Observed in Cresol-NO- $\text{NO}_x$  Air Runs.

$*$  = o-Cresol, EC-281  
 $\circ$  = m-Cresol, EC-289  
 $\Delta$  = p-Cresol, EC-290

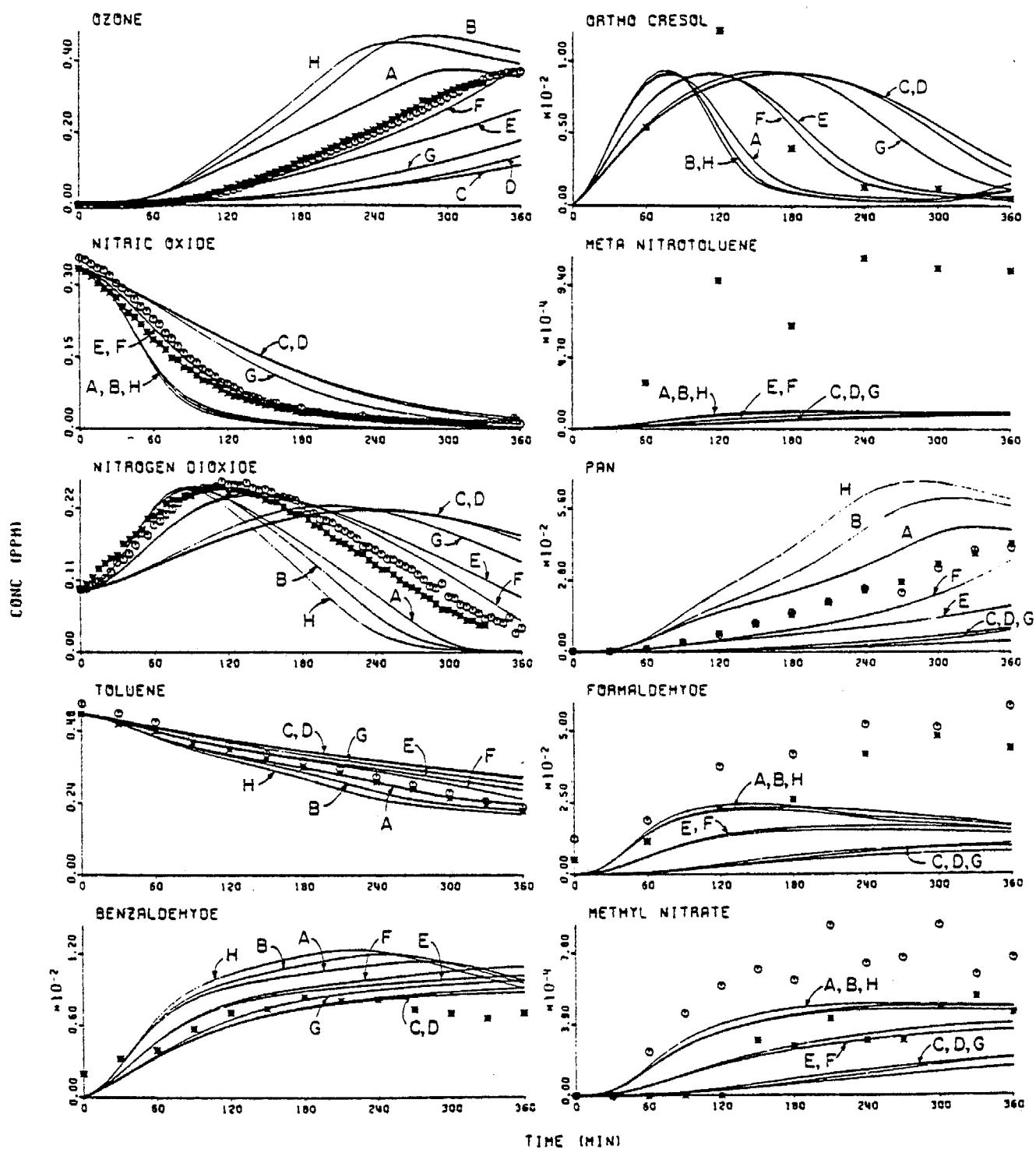


Figure 37. Experimental and Calculated Concentration-Time Profiles for Reactants and Products in Toluene-NO<sub>x</sub> Runs EC-327 and EC-340. Effect of Alternate Mechanisms for OH-Aromatic Adduct Fragmentations. ○ = Experimental Data, Run EC-327; \* = Experimental Data Run EC-340; — = Calculated, using Mechanisms A-H.

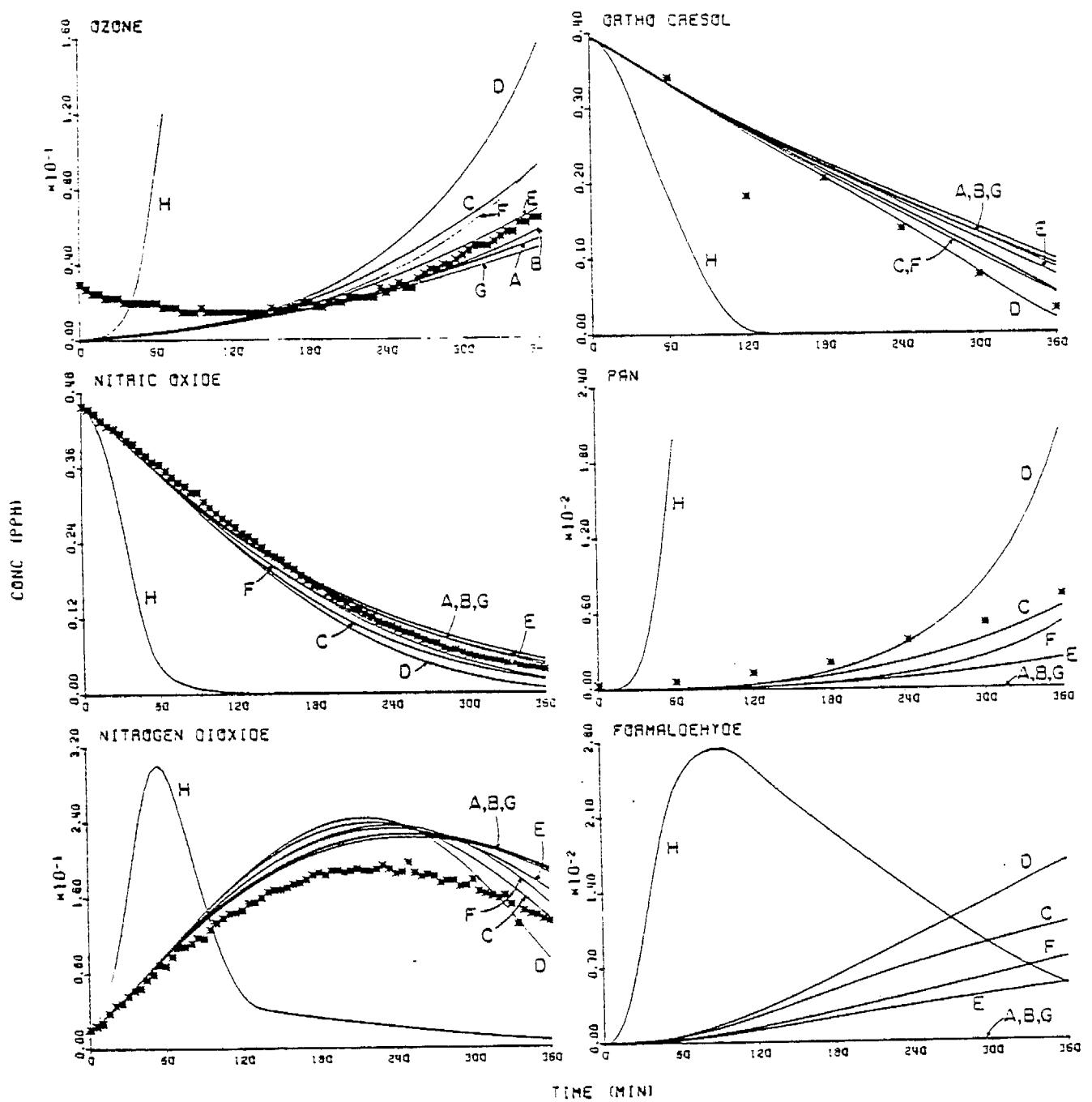


Figure 38. Experimental and Calculated Concentration-Time Profiles for Reactants and Products in o-Cresol- $\text{NO}_x$  Run EC-281. Effect of Alternate Mechanisms for OH-Aromatic Adduct Fragmentations.  
 \* = Experimental Data; — = Calculated using Mechanisms A-H.

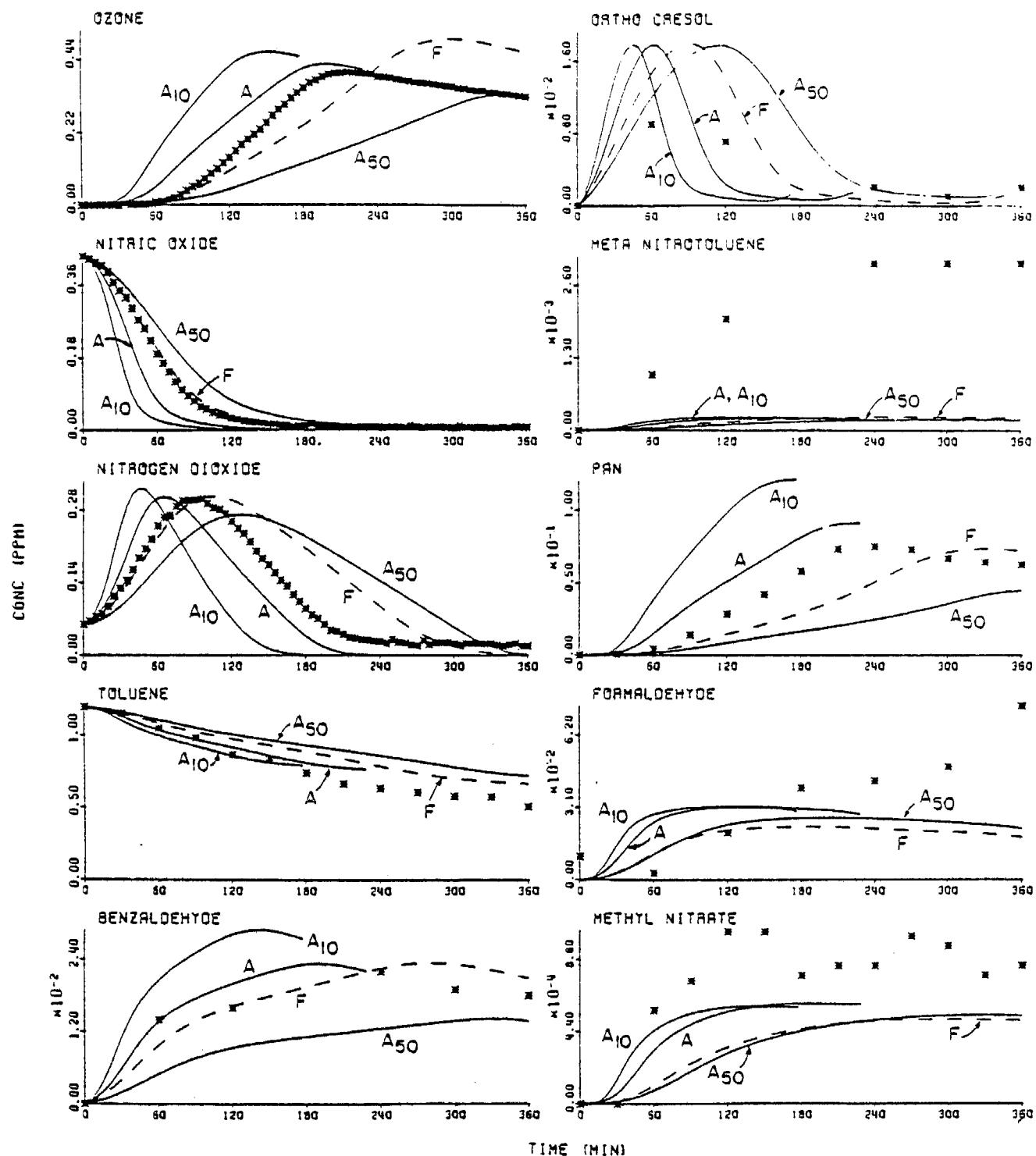


Figure 39. Experimental and Calculated Concentration-Time Profiles for Selected Reactants and Products in Toluene- $\text{NO}_x$  Run EC-266. Effect of Varying the Efficiency of Alkyl Nitrate Formation from  $\text{RO}_2 + \text{NO}_2$  from 10% (A<sub>10</sub>) to 50% (A<sub>50</sub>). \* = Experimental Data; — = Calculated.

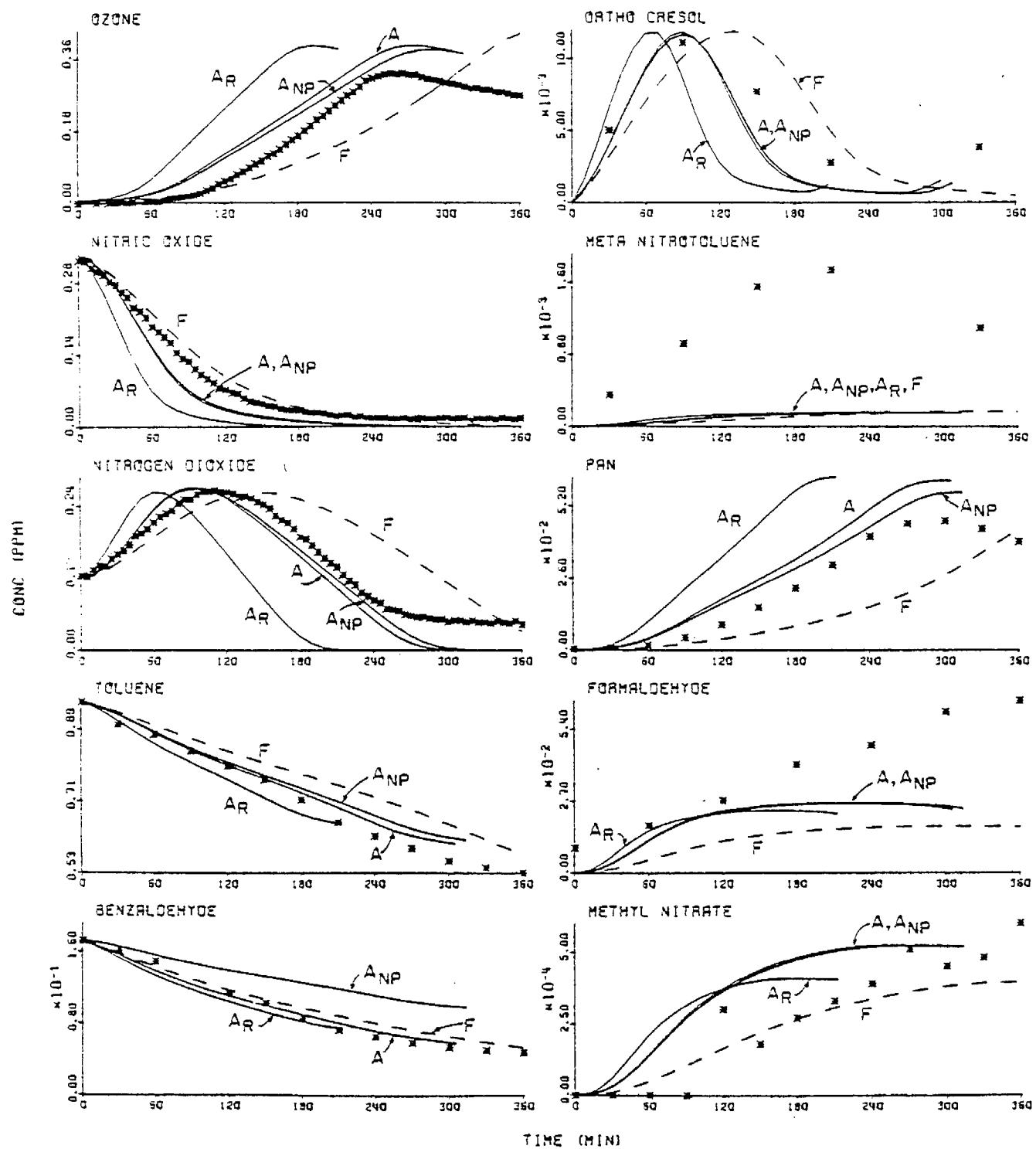


Figure 40. Experimental and Calculated Concentration-Time Profiles for Selected Reactants and Products in Toluene-Benzaldehyde-NO<sub>x</sub> Run EC-337. Effect of Assuming 100% Efficiency of Radical Production in Benzaldehyde Photolysis (AR), and Effect of Neglecting Benzaldehyde Photolysis (ANP). \* = Experimental Data; —, --- = Calculated.

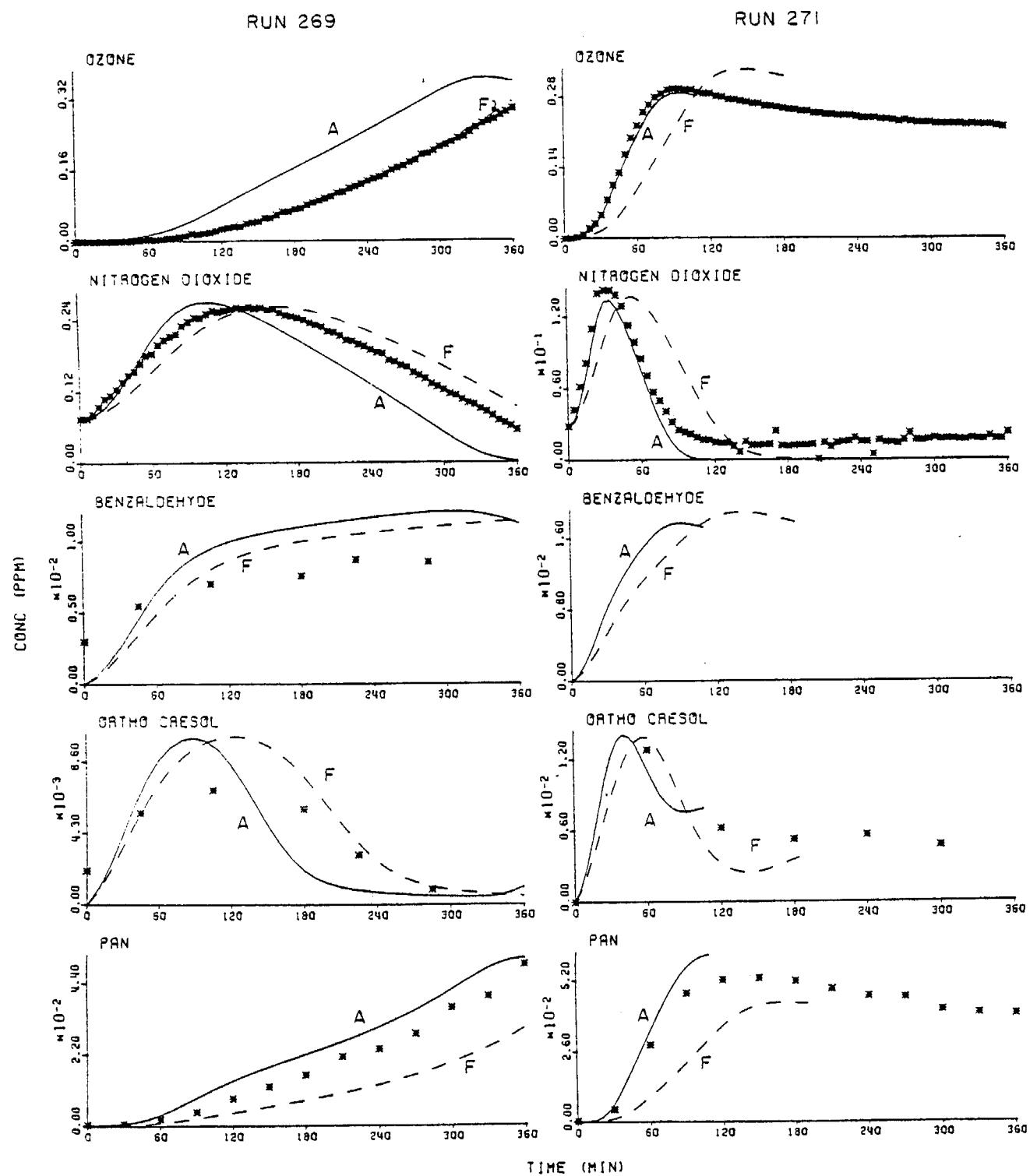


Figure 41. Experimental and Calculated Concentration-Time Profiles for Selected Reactants and Products in Toluene- $\text{NO}_x$  Runs EC-269 and EC-271. \* = Experimental Data; —, --- = Calculated.

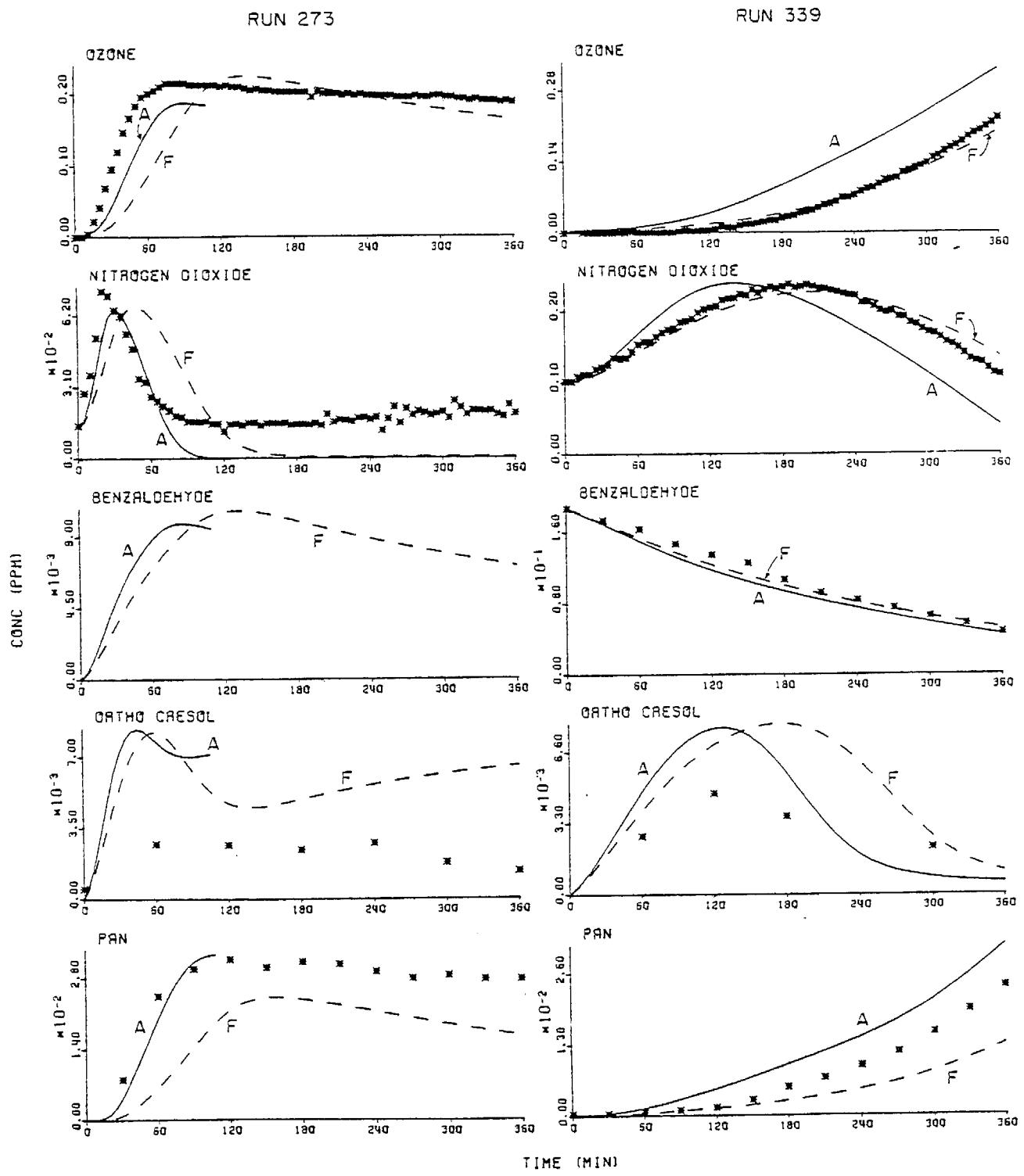


Figure 42. Experimental and Calculated Concentration-Time Profiles for Selected Reactants and Products in Toluene- $\text{NO}_x$  Run EC-273 and in Toluene-Benzaldehyde- $\text{NO}_x$  Run EC-339.  
 \* = Experimental Data; —, --- = Calculated.

ing light, are available from the Statewide Air Pollution Research Center upon request.

Results of Model Calculations. Calculations were carried out with varying mechanistic pathways and rate constant ratios. The various mechanistic options, which are described in more detail in the discussion, concern (a) the reactions of the species formed by the addition of hydroxyl radicals and then  $O_2$  to the aromatic ring, (b) the reactions of the predicted conjugated  $\gamma$ -dicarbonyl products, (c) the relative importance of the chain-terminating formation of organic nitrates from the  $RO_2 + NO$  reaction (e.g., reaction 38 and 4'), (d) the photolysis of benzaldehyde, and (e) the reaction of o-cresol with  $NO_3$  radicals. The varying assumptions made concerning these options, and the designation given the calculations using the different sets of assumptions, are given in Table 13.

Figure 37 and 38 show the effect of using different alternate mechanisms concerning the reactions of the OH-aromatic- $O_2$  adduct and the reactions of the  $\gamma$ -dicarbonyl products, compared with the experimental data for a representative toluene run and the o-cresol run; and Figure 39 shows the effect of varying the relative importance of the formation of nitrate from the  $RO_2 + NO$  reaction. From these figures, it can be seen that best fits are obtained if it is assumed that the aromatic-OH- $O_2$  adducts undergo cyclization but not re-cyclization (see discussion), and that the C<sub>7</sub> bicyclic peroxy radicals formed in the toluene and cresol photooxidations react with NO ~25% of the time to give nitrates. Both calculations A (assuming exclusively 3-addition of  $O_2$  to the aromatic-OH adduct, [2.2.2] cyclization of this aromatic-OH- $O_2$  adduct, and no cyclization of the  $RCH=CHCO_3$  radicals formed from the  $\gamma$ -dicarbonyl products) and calculations F ([3.2.1] cyclization of either the 1- $O_2^-$  or 3- $O_2^-$ -aromatic-OH adduct, and rapid cyclization of  $RCH=CHCO_3$ ) fit the data reasonably well, and the predictions of these two mechanisms are compared with the data from other toluene and toluene-benzaldehyde runs in Figures 39 - 42. In general, calculations A predict an initial reactivity which is slightly high, while calculations F predict a slightly low initial reactivity, although in both cases the calculated initial reactivity can be made to fit experimental results by respectively reducing or increasing the adjustable radical input rate from chamber sources (Carter et al., 1979)

Table 13

Sets of Mechanistic Options Examined in Model Calculations and Their Designation Symbols

Designation Symbol	Arom-OH-O <sub>2</sub> Adduct Formed	Arom-OH-O <sub>2</sub> Cyclization	Mechanistic Options					
			RCOCH=CHCO <sub>3</sub> Cyclization	k(C <sub>7</sub> O <sub>2</sub> +NO → C <sub>7</sub> ONO <sub>2</sub> ) k(C <sub>7</sub> O <sub>2</sub> +NO) Decomposition Mechanism	C <sub>6</sub> H <sub>5</sub> ClO Photolysis Mechanism	k(NO <sub>3</sub> +teresol) (cc-molecule <sup>-1</sup> sec <sup>-1</sup> )		
A	3-adduct <sup>a</sup>	[2, 2, 2] <sup>b</sup>	No <sup>c</sup>	No <sup>d</sup>	NA <sup>e</sup>	0.25	1.5 × 10 <sup>-11</sup>	Non-Radical
B	3-adduct	[2, 2, 2]	No	Yes	NA	0.25	1.5 × 10 <sup>-11</sup>	Non-Radical
C	1-adduct	[2, 2, 2]	No	No	NA	0.25	1.5 × 10 <sup>-11</sup>	Non-Radical
D	1-adduct	[2, 2, 2]	No	Yes	NA	0.25	1.5 × 10 <sup>-11</sup>	Non-Radical
E	NE <sup>f</sup>	[3, 2, 1]	No	No	NA	0.25	1.5 × 10 <sup>-11</sup>	Non-Radical
F	NE	[3, 2, 1]	No	Yes	NA	0.25	1.5 × 10 <sup>-11</sup>	Non-Radical
G	NE	NE	Yes	NA	$k'_1 >> k'_{33}$	0.25	1.5 × 10 <sup>-11</sup>	Non-Radical
H	NE	NE	Yes	NA	$k'_1 >> k'_{33}$	0.25	1.5 × 10 <sup>-11</sup>	Non-Radical
A <sub>10</sub>			Same as A			0.1	1.5 × 10 <sup>-11</sup>	Non-Radical
A <sub>50</sub>			Same as A			0.5	1.5 × 10 <sup>-11</sup>	Non-Radical
A <sub>R</sub>			Same as A			0.25	1.5 × 10 <sup>-11</sup>	Radical
A <sub>NP</sub>			Same as A			0.25	1.5 × 10 <sup>-11</sup>	No Photolysis
A <sub>NN</sub>			Same as A			0.25	1.5 × 10 <sup>-11</sup>	Non-Radical

<sup>a</sup>3-adduct:  $k_{45} \gg k_{44}$  (toluene system);  $k_{69} \gg k_{68}$  (teresol system); 1 adduct:  $k_{44} \gg k_{45}, k_{68} \gg k_{69}$ .<sup>b</sup>Refers to structure of bicyclic ring system. [2, 2, 2]:  $k'_1 > k'_7$ ; [3, 2, 1]:  $k'_7 >> k'_1$ .<sup>c</sup>Yes:  $k'_{16} >> k'_3[\text{NO}]$  or  $k'_{17} >> k'_9[\text{NO}]$  or  $k'_{18} >> k'_{11}[\text{NO}]$ ; No:  $k'_{16}, k'_{17}, k'_{18}$  negligible.<sup>d</sup>Yes:  $k_{108} \gg (k_{110}[\text{NO}] + k_{112}[\text{NO}_2])$  and  $k_{109} \gg (k_{111}[\text{NO}] + k_{113}[\text{NO}_2])$ ; No:  $k_{108}, k_{109}$  negligible.<sup>e</sup>NA = Not applicable. Intermediates involved not formed in this set of options.<sup>f</sup>NE = No effect. The same intermediates or products are formed regardless of the assumptions made.

(see note 8 of Appendix A).

Figure 40 shows the effect on model calculations of varying assumptions concerning benzaldehyde photolysis for a toluene-benzaldehyde run. It can be seen that in order to fit the benzaldehyde concentration-time profiles and the overall reactivity, it is necessary to assume that benzaldehyde undergoes photolyses at a significant rate, but that it forms non-radical products.

Figure 43 shows the effect that a reaction of  $\text{NO}_3$  with o-cresol has on the  $\text{O}_3$ ,  $\text{NO}_2$  and o-cresol concentration-time profiles in the o-cresol run and in a toluene-benzaldehyde run. Predicted concentration-time profiles of other monitored reactants and products are less affected by this reaction. It can be seen that the data are much better fit by assuming that the reaction occurs with a rate constant on the order of  $(1-2) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ sec}^{-1}$  than by assuming it is negligible.

Table 12 lists the experimental and calculated (using model A) yields of the major products monitored, and gives the maximum calculated yields of major products predicted by the model which were not experimentally monitored. Among the products monitored the major discrepancy appears to be that the observed nitrotoluene yields are higher by a factor of ~10 than those calculated, despite the fact that the calculations generally fit the cresol data and used the experimentally determined ratio ( $k_{42}/k_{43}$ ) for cresol vs. nitrotoluene formation obtained by Kenley et al. (1978). In addition, the predicted formaldehyde yields are slightly low, relative to the experimental data. This may be due to the neglect of glyoxal photolysis in our mechanism (see note 29). For the other major products, the fits of calculated to experimental yields can be considered to be within the range of the experimental uncertainties. Although the model predicts the formation of products which were not experimentally observed (mainly C<sub>7</sub> organic nitrates,  $\alpha$ -dicarbonyls, 2-butene-1,4-dial, peroxybenzoyl nitrate (PBzN) and nitrophenols), we have no evidence that these species are not formed in the yields predicted. Indeed, the low carbon balance observed for these systems suggests a significant formation of unmonitored products, and thus, except for the nitrotoluene yields (a very minor product) our model simulations can be considered to be generally consistent with the experimental data reported here.

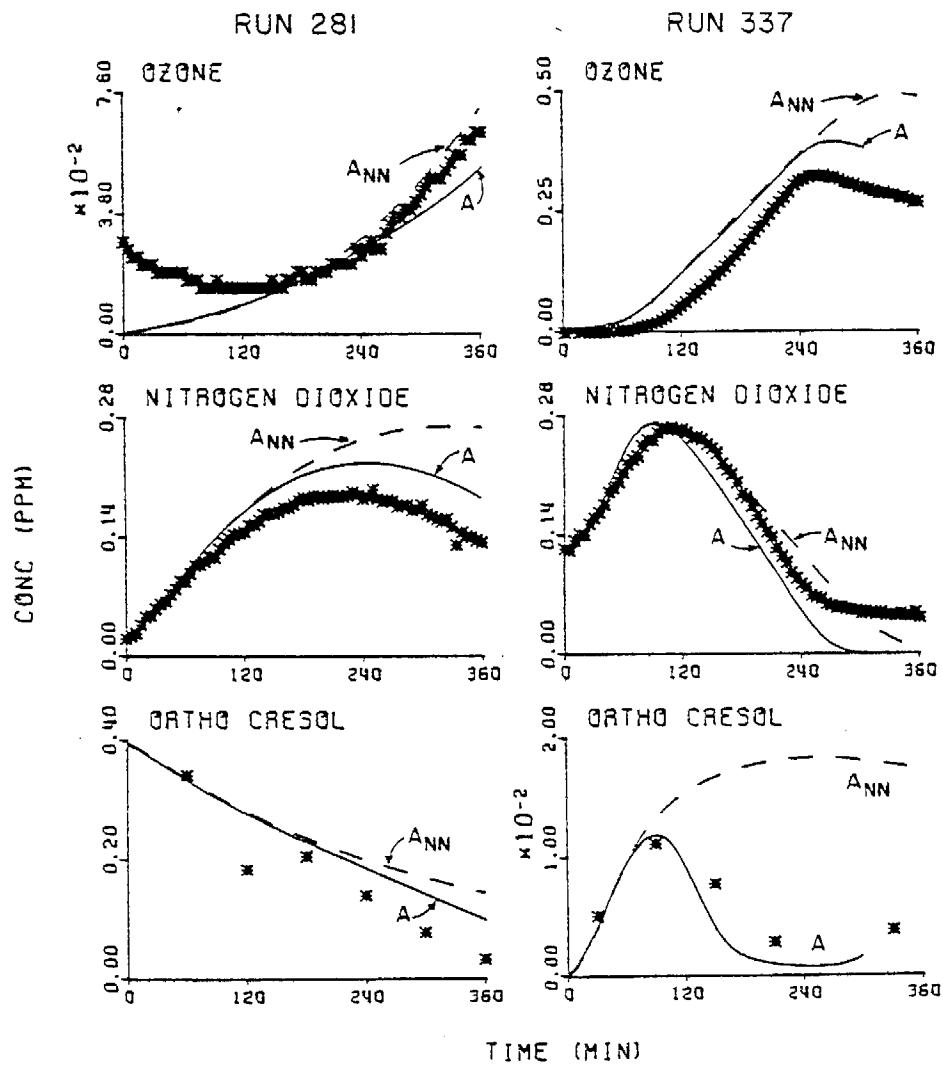
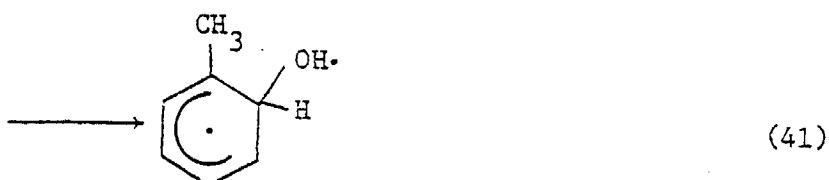
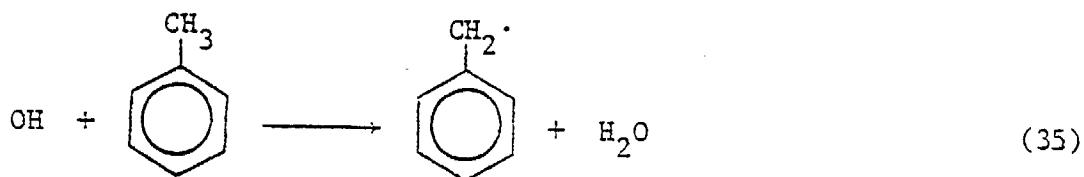


Figure 43. Experimental and Calculated Concentration-Time Profiles for  $\text{O}_3$ ,  $\text{NO}_2$ , and o-Cresol in o-Cresol- $\text{NO}_x$  Run EC-281 and in Toluene-Benzaldehyde- $\text{NO}_x$  Run EC-337. Effect of Neglecting the  $\text{NO}_3 + \text{o-Cresol}$  Reaction (ANN). \* = Experimental Data; —, --- = Calculated.

Discussion.

1. Initial Toluene Reactions. The only significant chemical loss process of toluene under simulated polluted atmospheric conditions is now known to be by reaction with the OH radical (Hendry et al., 1978; Atkinson et al., 1979; Doyle et al., 1975; Davis et al., 1975; Hansen et al., 1975; Lloyd et al., 1976; Perry et al., 1977a; Ravishankara et al., 1978; Kenley et al., 1978; Hendry, 1979; Pate et al., 1976a).

This reaction proceeds via two pathways: H atom abstraction from the substituent methyl group (reaction 35), and OH radical addition to the ring (reaction 41) (Hendry et al., 1978; Atkinson et al., 1979; Davis et al., 1975; Perry et al., 1977a; Ravishankara et al., 1978; Kenley et al., 1978; Hendry, 1979; O'Brien, 1975; Spicer and Jones, 1977; Hoshino et al., 1978; Grosjean et al., 1978; O'Brien et al., 1979; Akimoto et al., 1978),

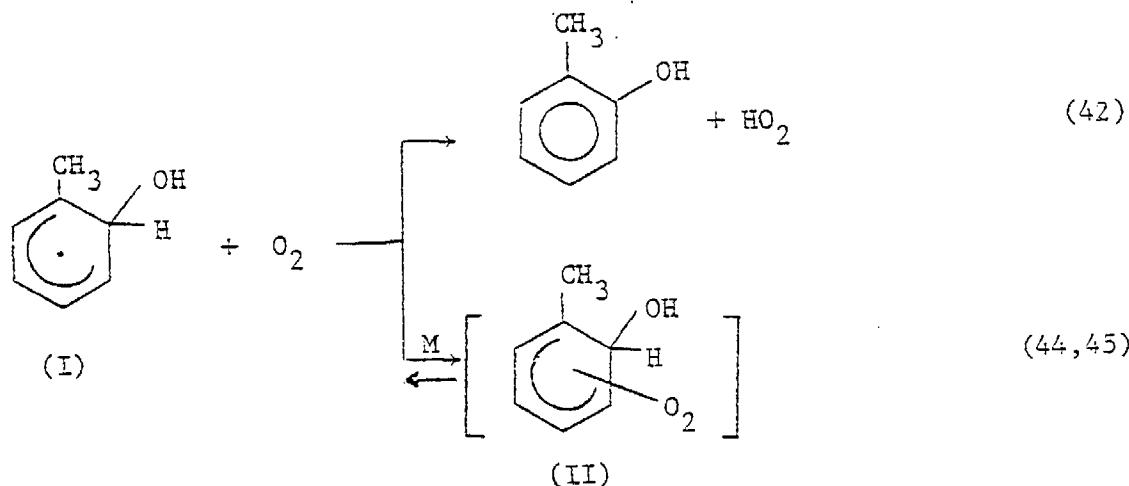


with  $k_{35}/(k_{35} + k_{41}) \approx 0.15$  (Atkinson, et al., 1979; Perry et al., 1977a; Kenley et al., 1978; Hendry, 1979) and  $(k_{35} + k_{41}) \approx 6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ sec}^{-1}$  (Atkinson et al., 1979; Davis et al., 1975; Hansen et al., 1975; Perry et al., 1977a) at room temperature. Under atmospheric conditions the benzyl radical will react to form benzaldehyde and benzyl nitrate (reactions 36-40), as has been discussed previously (Hendry et al., 1978; Atkinson et al., 1979; Kenley et al., 1978; Hendry, 1979; O'Brien, 1975; Spicer and Jones, 1977; Hoshino et al., 1978; Grosjean et al., 1978;

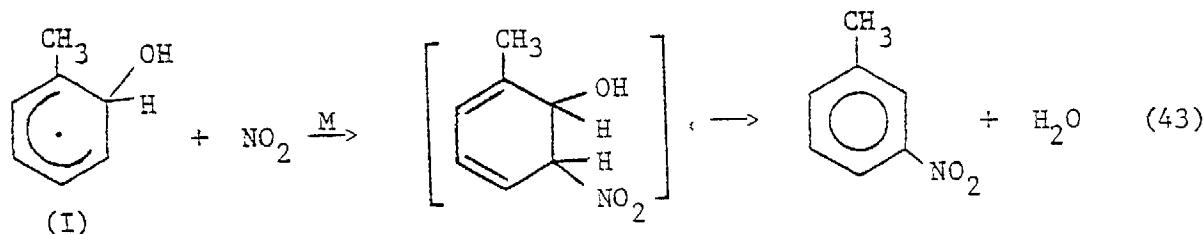
O'Brien et al., 1979). The reasonably good fits of the model calculations to the experimental benzaldehyde yields (see Table 12) indicate that our data is consistent with the reported ratios (Atkinson et al., 1979; Perry et al., 1977a; Kenley et al., 1978; Hendry, 1979) for OH abstraction of hydrogen vs. OH radical addition to the aromatic ring.

OH Radical Addition Pathway: Formation of Cresols and Nitrotoluene.

The major pathway (~85%) for reaction of OH radicals with toluene is via the initial formation of an OH-toluene adduct (Atkinson et al., 1979; Perry et al., 1977a; Kenley et al., 1978; Hendry, 1979). By analogy with the position of O(<sup>3</sup>P) atom addition to toluene (Jones and Cvetanovic, 1961; Grovenstein and Mosher, 1970; Gaffney et al., 1976) and based on the available experimental product data (Kenley et al., 1978; Hendry, 1979; O'Brien, 1975; Hoshino et al., 1978; Grosjean et al., 1978; O'Brien et al., 1979; Akimoto et al., 1978), the OH radical is presumed to add primarily at the ortho position. The thermalized adduct (I) can react under atmospheric conditions with O<sub>2</sub> via two pathways (Atkinson et al., 1979): H atom abstraction to form the cresol (reaction 42), or reversible addition to form the peroxy radical (II) (reaction 44, 45):



or it can react with NO<sub>2</sub> to form the nitrotoluene:

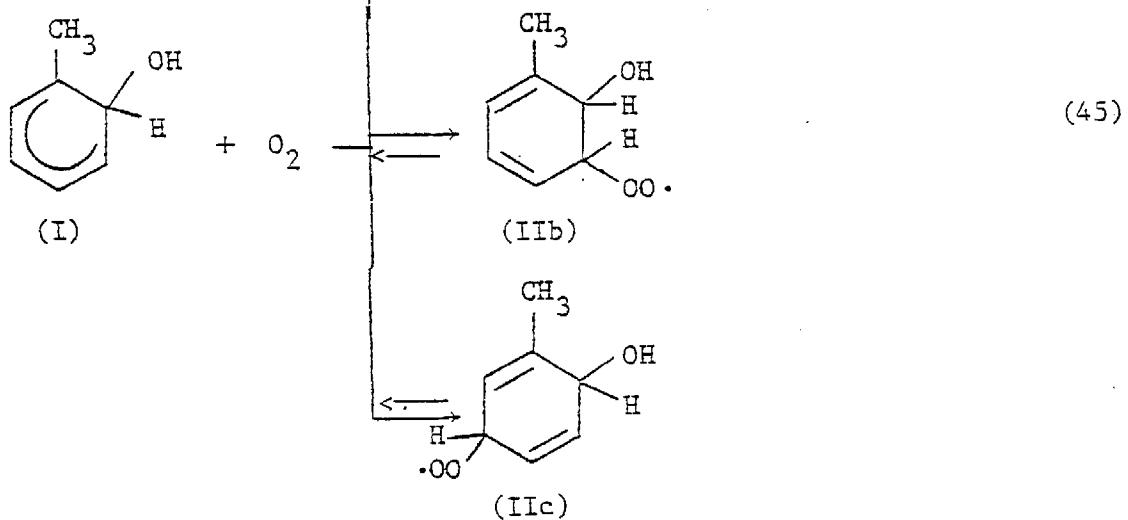
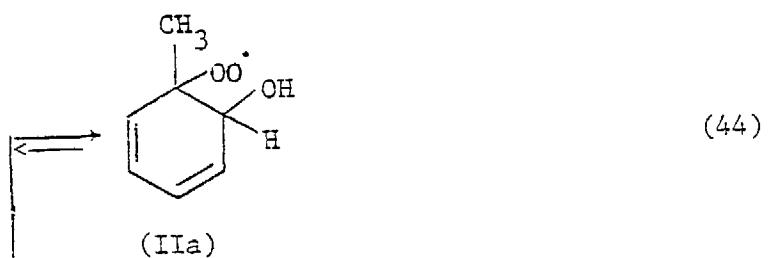


Hendry and co-workers (Kenley et al., 1978; Hendry, 1979) concluded from their discharge flow study of the reaction of OH radicals with toluene that the cresol isomers and m-nitrotoluene (i.e., reaction 42 and 43) are the sole initial products of the OH radical addition pathway, and that  $k_{43}/k_{42} = (4.4 \pm 0.5) \times 10^3$ . If the discharge-flow results (Kenley et al., 1978; Hendry, 1979) are applicable to the present experimental study, the only significant initial products of toluene photooxidation would be benzaldehyde and the cresols, with the latter being formed ~85% of the time. Because the cresols are consumed more rapidly in the  $\text{NO}_x$ -air irradiations than toluene, due to their higher rate constant for reaction with the OH radical (Atkinson et al., 1979; Perry et al., 1977b; Atkinson et al., 1978b) this would mean that the chemistry of the toluene- $\text{NO}_x$  system would be dominated by that of the cresol- $\text{NO}_x$  system. However, the present smog chamber results indicate that in terms of ozone and PAN formation and NO to  $\text{NO}_2$  conversion rates, the cresol- $\text{NO}_x$ -air systems are far less reactive than the toluene system. The excess reactivity of the toluene system cannot be attributed to benzaldehyde reactions, since, as is discussed below, benzaldehyde acts as an inhibitor (Gitchell et al., 1974; Niki et al., 1978; Niki et al., 1979). Thus the initial formation of products other than these is necessary to account for the relatively high reactivity of toluene runs, and for the high yields of products such as PAN, as well as for the observation of biacetyl as an initial product in o-xylene- $\text{NO}_x$ -air irradiations (Darnall et al., 1979). We find the o-cresol data is best fit by assuming it is formed to the extent of only ~20% of the total OH + toluene reaction, with products other than cresol, benzaldehyde, benzyl nitrate and nitrotoluenes being formed ~65% of the time.

The apparent inconsistency in terms of predicted cresol and nitrotoluene yields between the results of the discharge flow studies (Kenley et al., 1978) and our smog chamber studies may be due to the fact that the former was carried out at a total pressure of ~6-15 torr of (Ar +  $\text{O}_2$ ) (Kenley et al., 1978) against a total pressure of 1 atm of air in the smog chamber studies.  $\text{O}_2$  addition to (I) to form (II) and the reaction of (I) with  $\text{NO}_2$  to form nitrotoluenes both may have not been in the limiting high pressure second order kinetic regime under the conditions of the discharge-flow study (Kenley et al., 1978), and thus could be significantly

faster at 1 atm total pressure. This is indeed assumed to be the case for the addition reaction of (I) with  $O_2$ , but the model still uses the low pressure-derived value for the (I) +  $NO_2$  addition reaction (reaction 43). However, the fact that the model significantly underpredicts nitrotoluene yields suggests that  $k_{43}$  is pressure dependent as well.

Structure and Reactions of the OH-Aromatic- $O_2$  Adducts. The structure of the radical (II) is not known; addition of  $O_2$  to (I) may be at the 1-, 3-, or 5-position:

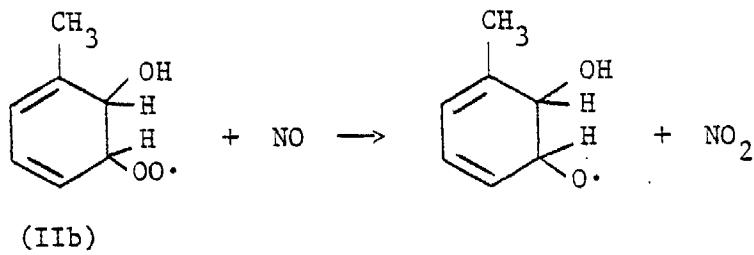


$O_2$  addition at the 5-position should be the least thermodynamically favored, since the double bonds are nonconjugated. Addition at the 1-position (reaction 44) is estimated (Benson, 1976) to be slightly more favored thermodynamically over addition to the 3-position (reaction 45), although the resulting radical (IIa) will also have the most steric hindrance. In the calculations, the consequences of assuming exclusively 1-addition or exclusively 3-addition are both considered.

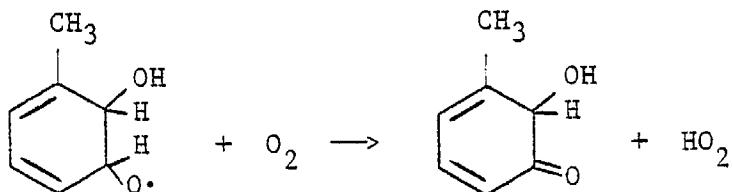
Based on thermochemical estimates (Perry et al., 1977a; Benson, 1976),  $O_2$  addition to radical I is expected to be only  $\sim 10$  kcal mole $^{-1}$  exothermic. This means that significant back-decomposition of radicals II to radical I may be occurring, which could account for the relatively low effective rate constant for  $O_2$  addition to radical I required to fit the cresol data (see note 13, Appendix A).

At the present time little is known about the other reaction pathways of the OH-aromatic- $O_2$  adducts. There are a number of possible alternative pathways, and these are listed for a general aromatic adduct in Appendix B and are discussed below for the case of adduct IIb (substituent 6 in Appendix B = CH<sub>3</sub>, substituents 1-5 = H). Reactions of the other adducts are assumed to be analogous.

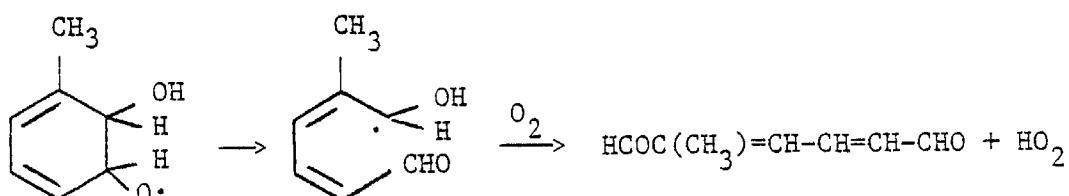
If the OH-aromatic- $O_2$  adducts react in a manner analogous to other peroxy radicals, the following scheme would appear to be the most reasonable:



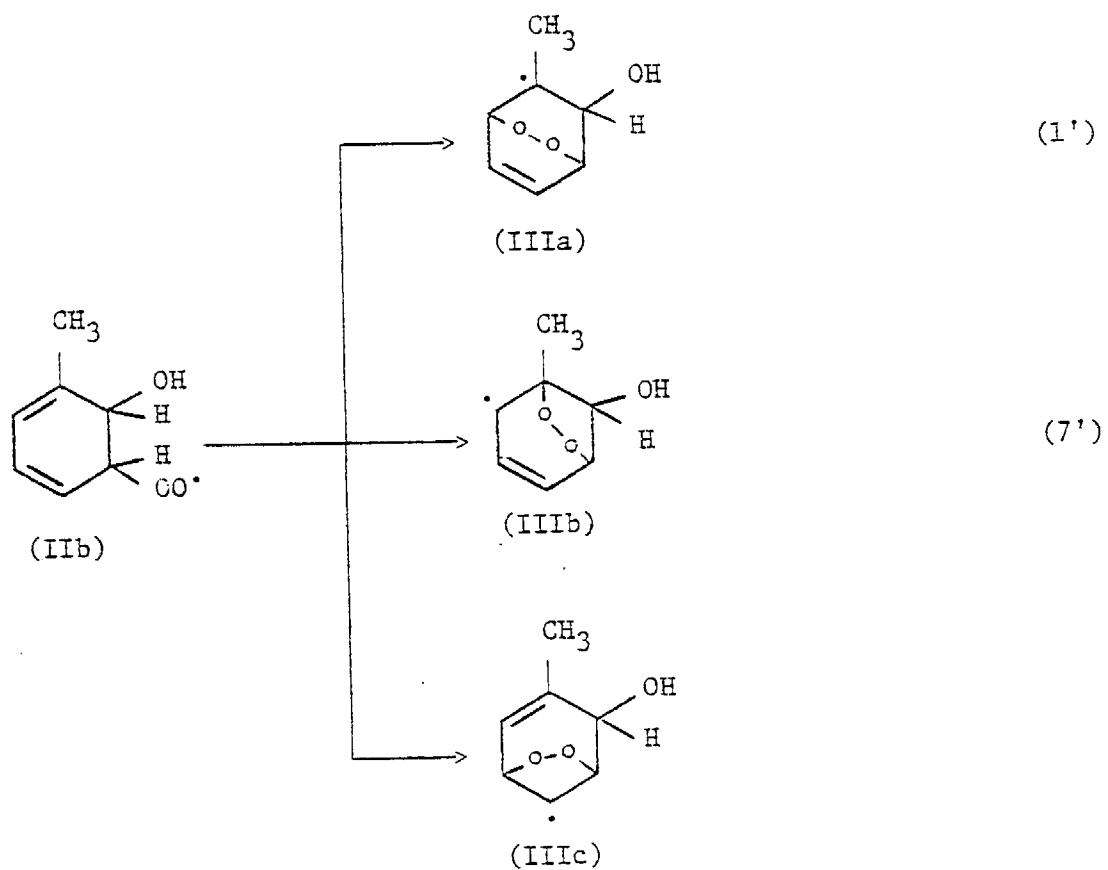
followed by either reaction with  $O_2$



or ring opening



However, this scheme is inconsistent with the observation of biacetyl as a primary product in the  $\text{NO}_x$ -*o*-xylene-air system (Darnall et al., 1979), and no reasonable mechanism accounting for that observation (Darnall et al., 1979) could be derived without assuming formation of bicyclic radicals. It is thus assumed that the OH-aromatic- $\text{O}_2$  adduct primarily undergoes cyclization reactions such as those shown below:

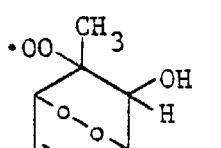


In addition to accounting for the ring cleavage products observed, these reactions are expected to dominate on the basis of thermochemical and kinetic estimates. If we assume that the rate constant for the reaction of the peroxy radical IIb with NO is  $\sim 8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ sec}^{-1}$  (see note 9 of Appendix A), then under realistic atmospheric conditions  $[\text{NO}] < 1 \text{ ppm}$  ( $2 \times 10^{13} \text{ molecule cm}^{-3}$ ) cyclization should dominate if its rate constant is  $> 160 \text{ sec}^{-1}$ . If we further assume that (1) the A factors for the cyclization reactions are at a minimum  $\sim 10^{10} \text{ sec}^{-1}$  (Benson, 1976), (2) that the

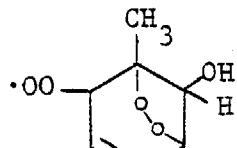
activation energy for cyclization is [ $\leq$  9 kcal mole<sup>-1</sup> (based on the activation energies of bimolecular radical + double bond addition reactions [Kerr and Parsonage, 1972]) + the reaction endothermicity (if any)] and (3) that  $\Delta H$  (cyclization)  $\approx$  (ring strain-14) kcal mole<sup>-1</sup>, based on thermochemical calculations using group additivity principles (Benson, 1976), then cyclization should dominate if the ring strain of the bicyclic radicals is less than ~16 kcal mole<sup>-1</sup>. Although such ring strains are not known, this would appear to be likely (Benson, 1976).

Of the radicals IIIa-c, IIIa will probably have the least ring strain, while IIIb will have some resonance stabilization energy by virtue of its allylic character. Since we cannot determine, *a priori*, which of these structures is favored, it is again necessary to consider both options in the model calculations, i.e. IIIa or IIIb.

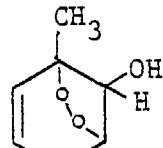
These cyclized aromatic-OH-O<sub>2</sub> adducts are then expected to add O<sub>2</sub> to form radicals of the type



IV

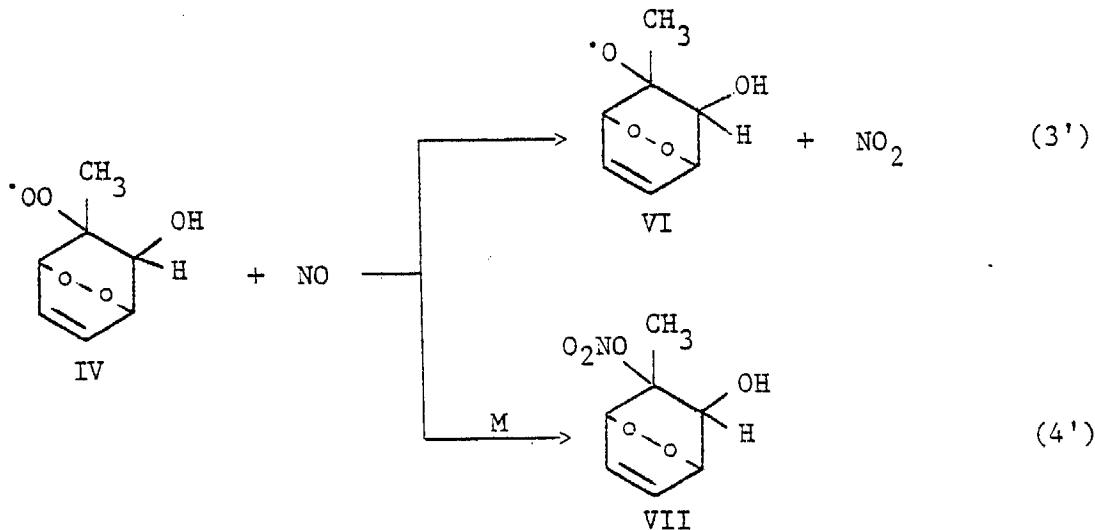


Va

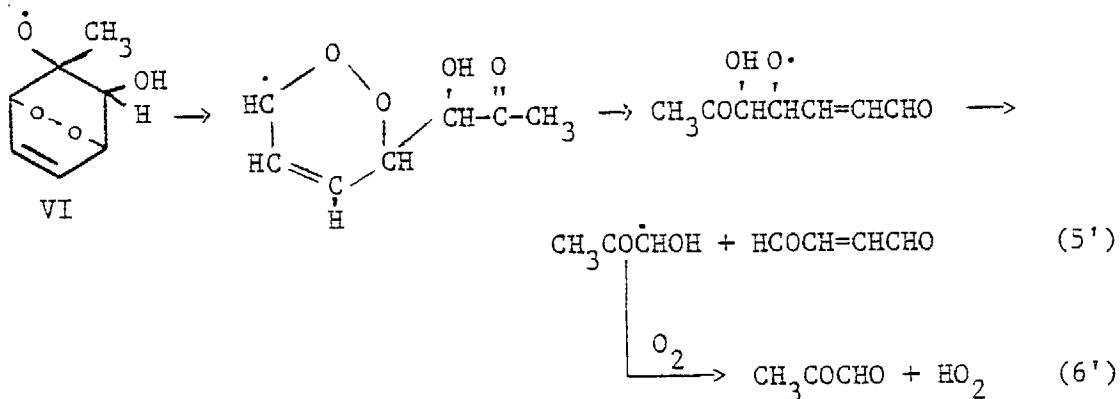


Vb

which could react with NO either to form an alkoxy radical or yield a stable nitrate (analogous to the  $\geq C_4$  alkylperoxy cases [Carter et al., 1979]), for example:

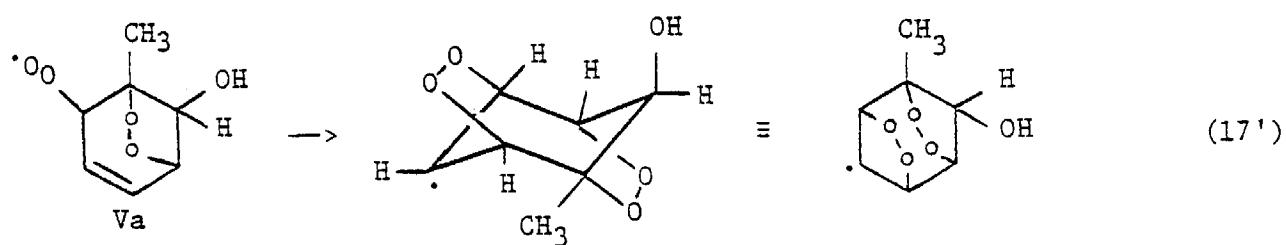
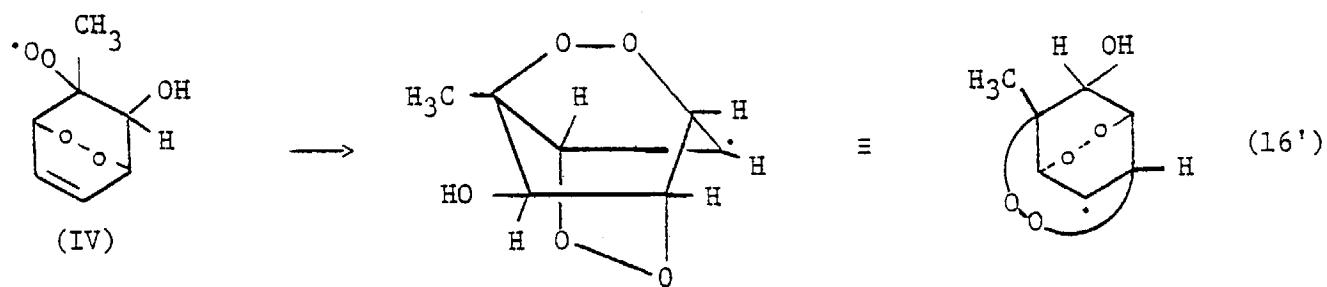


The reactions of the bicyclic peroxy organic nitrates such as (VII) are unknown; they may undergo molecular decomposition to form  $\text{HNO}_3$  or other organic nitrates. In our model we assume their reactions, if any, have a negligible effect on the overall mechanism and are thus ignored. The bicyclic peroxy alkoxy radicals such as (VI) are expected to undergo a series of highly favorable  $\beta$ -scission fragmentations, resulting in the formation of  $\alpha$ -dicarbonyl and conjugated  $\gamma$ -dicarbonyl products. For example, (VI) is assumed to decompose as shown, with the other isomers, resulting from the reaction of NO with Va and Vb, reacting analogously:

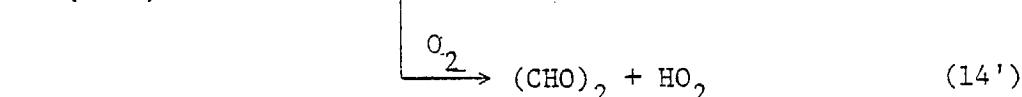
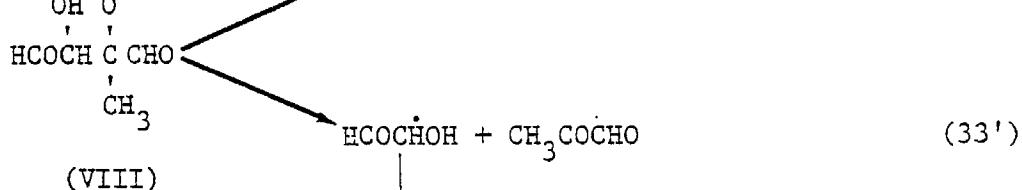
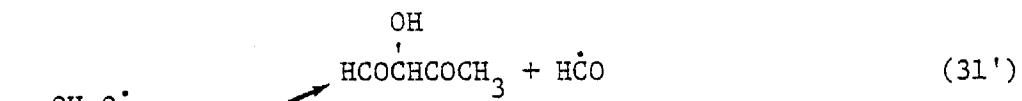
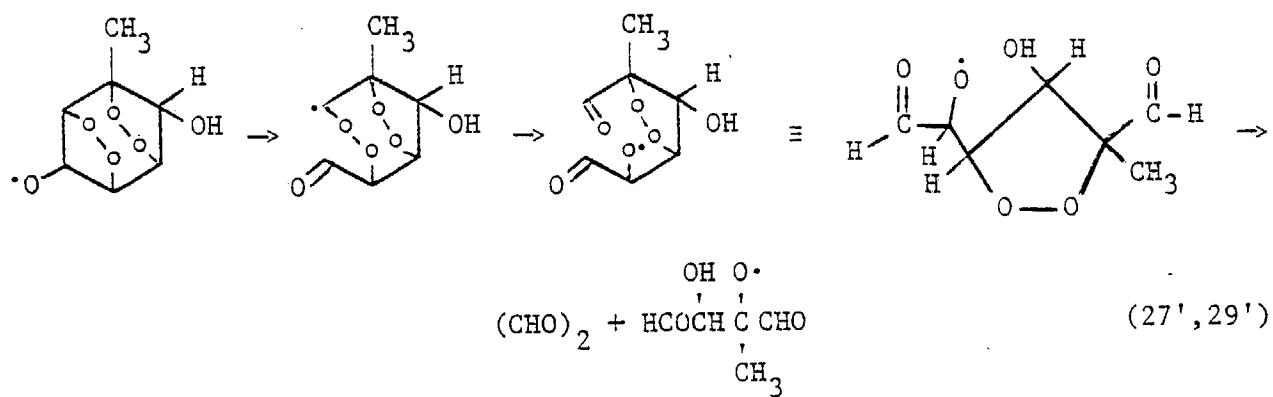


The relative importance assumed for nitrate formation vs. alkoxy radical formation has an important effect on model simulations, since the former process is radical terminating and is an effective nitrogen sink, while the latter is radical propagating. This effect is shown in Figure 39, where  $k_4'/(k_3' + k_4')$  (and also the analogous rate constant ratios in the cresol system and for the benzyl peroxy radical) is varied from 0.1 to 0.5. It can be seen that toluene- $\text{NO}_x$ -air data is best fit by assuming nitrate formation occurs ~25% of the time; this is true for the toluene-benzaldehyde- $\text{NO}_x$ -air and the cresol- $\text{NO}_x$ -air system as well. Assuming nitrate formation is negligible results in a significant overproduction at ozone maxima regardless of the other mechanistic options used.

A possibility which must also be considered is that the bicyclic peroxy radicals may further cyclize, such as shown below (for radical (IV) and the  $\text{O}_2$  adduct to radical (IIIb)):



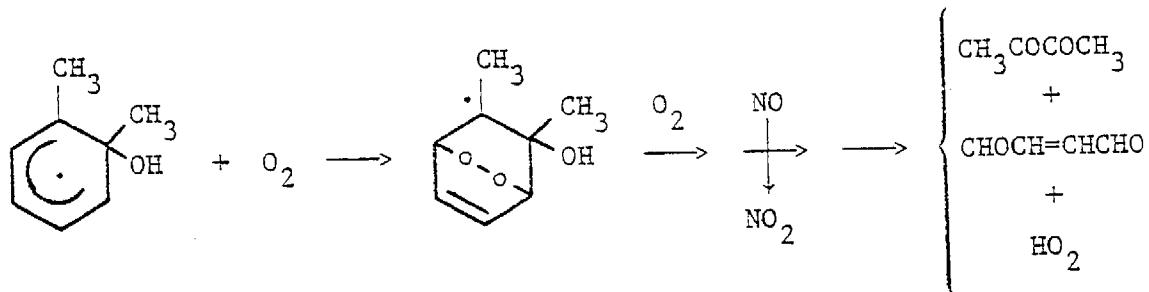
If formed, these double cyclized radicals should react with  $O_2$  and then NO forming alkoxy radicals or alkyl nitrates by reactions analogous to those shown above for (IV). The tricyclic bridged-peroxy alkoxy radicals are also expected to rapidly fragment via consecutive  $\beta$ -scissions:



The relative importance of the two possible modes of decomposition (e.g., reaction 31' and 33') of species such as (VIII) is not known so both possibilities are considered.

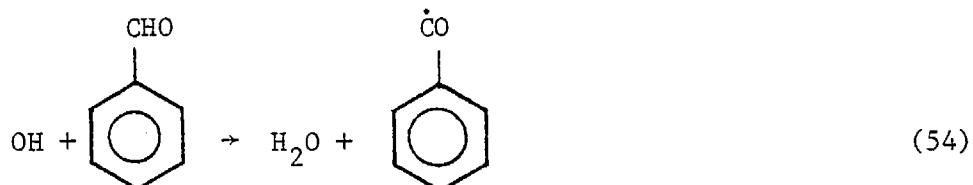
As can be seen from Figures 37 and 38, the data do not clearly indicate which aromatic-OH-O<sub>2</sub> adduct is formed or whether it undergoes [2.2.2] or [3.2.1] cyclization, but do indicate that recyclization probably is negligible. If recyclization occurs, the assumption made concerning the fragmentation of radical (VIII) is important (assuming reaction 33' dominates results in over-prediction of reactivity in the toluene and the o-cresol systems, while assuming reaction 31' dominates results in the reactivity in the toluene system being underpredicted, but gives reasonably good fits to the o-cresol system); but it is clear that no adjustment of the k<sub>31'</sub>/k<sub>33'</sub> ratio would allow both the toluene-NO<sub>x</sub> data and the o-cresol-NO<sub>x</sub> data to be fit by models assuming recyclization. Model (A) assumes [2.2.2] cyclization and predominant addition of O<sub>2</sub> to the 1-position of the OH-aromatic adduct, although 3-addition should not be completely negligible. If [3.2.1] cyclization occurs, as assumed in the other model which gives reasonable fits to the data (F), formation of the 1-adduct or the 3-adduct is immaterial, since each cyclize to form the same intermediate (i.e., radical IIIb).

The aromatic ring-opening mechanisms which best fit the toluene and o-cresol data, when applied to the o-xylene system, yield biacetyl after OH radical addition at the 1- or 2-position, for example:



This is, as noted previously, in accord with the recent observation of significant yields ( $18 \pm 4\%$ ) of biacetyl from irradiated NO<sub>x</sub>-o-cresol-air systems (Darnall et al., 1979) and the magnitude of the biacetyl yield is then consistent with the mode of O(<sup>3</sup>P) atom addition to o-xylene (Grovenstein and Mosher, 1970).

Benzaldehyde Reactions. The reaction of benzaldehyde with OH radicals must, because of the magnitude of the OH radical rate constant (Niki et al., 1978), proceed predominately via H atom abstraction from the substituent CHO group (Hendry et al., 1978; Atkinson et al., 1979; Hendry, 1979) to form the benzoyl radical:

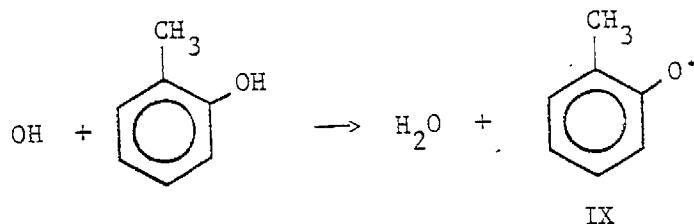


This  $\text{C}_6\text{H}_5\text{CO}$  radical is then expected to add  $\text{O}_2$  (reaction 56) to form the peroxybenzoyl radical which can react with NO or  $\text{NO}_2$ . Reaction with  $\text{NO}_2$  (reaction 57) will lead to the formation of peroxybenzoynitrate (PBzN), which was not observed, but which may have been formed and not detected. PBzN thermally decomposes (Hendry and Kenley, 1979) with an analogous mechanism to PAN (Pate et al., 1976b; Hendry and Kenley, 1977; Cox and Roffey, 1977) to lead to the ultimate formation of, among other products, o- and p-nitrophenols (reactions 58-65) (Niki et al., 1979). Note that in each case the ultimate result of the OH-benzaldehyde reaction is radical termination, which is consistent with these and previously reported observations (Gitchell et al., 1974; Niki et al., 1978; Niki et al., 1979).

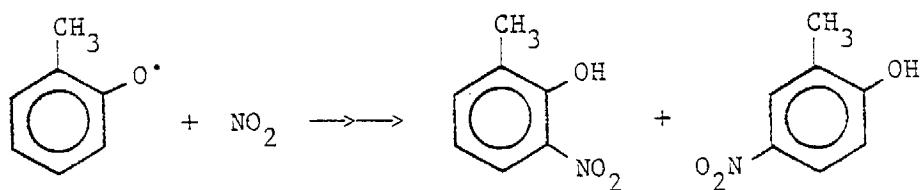
While little is known about benzaldehyde photolysis under atmospheric conditions, its photolysis at rates approximately 5 times greater than that used for the aliphatic aldehydes (Carter et al., 1979) is included in the mechanism to account for the observed benzaldehyde loss rates in the toluene-benzaldehyde runs (see note 20 of Appendix A). As noted previously (see Figure 40), the data are best fit by assuming that benzaldehyde photolysis results in the formation of nonradical products. The most likely pathway would thus appear to be formation of benzene + CO, but although small yields of benzene (~0.5-1 ppb) are indeed observed in the toluene-benzaldehyde runs, the yields are far less than the amounts predicted (50-60 ppb) if it were the major product of benzaldehyde photolysis.

Cresol Reactions. The cresols, represented in this model by o-cresol alone (substantiated to a large extent by the smog chamber data reproduced here), are known to react rapidly with OH radicals (Atkinson et al., 1979; Perry et al., 1977b; Atkinson et al., 1978b), with this reaction being a major cresol loss process under simulated atmospheric conditions (Atkinson et al., 1978b). The slow reaction with O<sub>3</sub> (Atkinson et al., 1978b; Hendry, 1979) has been neglected in the present model since it will contribute <5-10% of the total cresol loss rate under the experimental conditions employed in the NO<sub>x</sub>-toluene-air and NO<sub>x</sub>-o-cresol-air irradiations. The irradiated NO<sub>x</sub>-o-cresol-air data yields little evidence as to the reaction mechanisms--very little PAN is formed and the major organic products observed are hydroxynitrotoluenes in low (< 5%) yields. The reaction of OH radicals with o-cresol can proceed via OH radical addition to the ring or by H atom abstraction (Atkinson et al., 1979; Perry et al., 1977b).

The abstraction pathway, which accounts for ~8% of the total OH radical reaction (Atkinson et al., 1979), probably proceeds mainly via H atom abstraction from the substituent-OH group, since the abstraction rate constant for o-cresol is a factor of ~4 higher at 400 K than that for toluene (Perry et al., 1977a; 1977b).

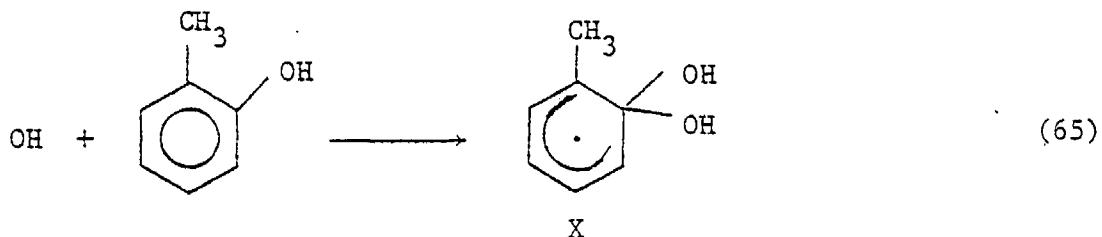


Reactions of NO<sub>2</sub> with radical IX can, by analogy to the phenoxy radical reaction 64 (Niki et al., 1979), lead to formation of the observed hydroxynitrotoluene isomers. This minor H atom abstraction pathway has been

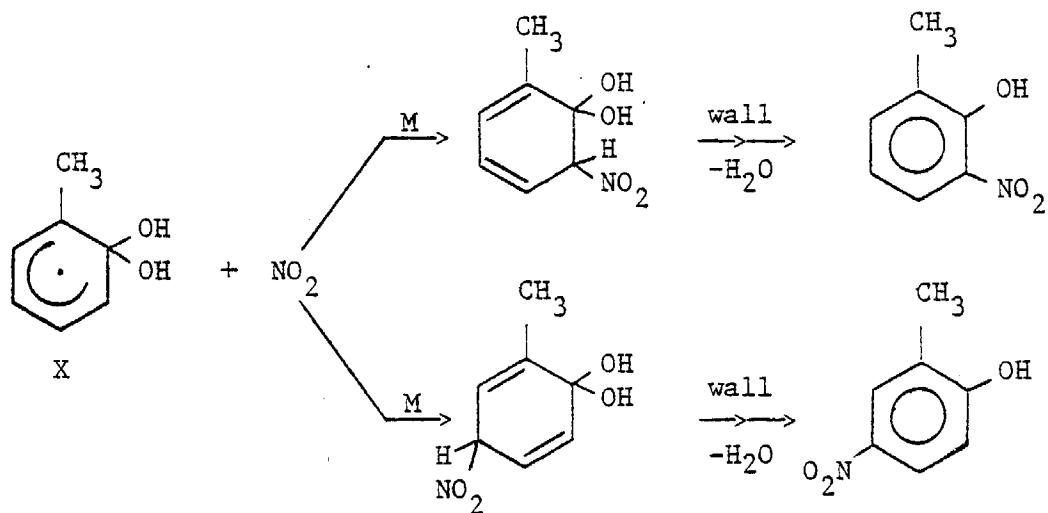


neglected in the model calculations since its inclusion would have an insignificant effect on the calculated time-concentration profiles of the major species.

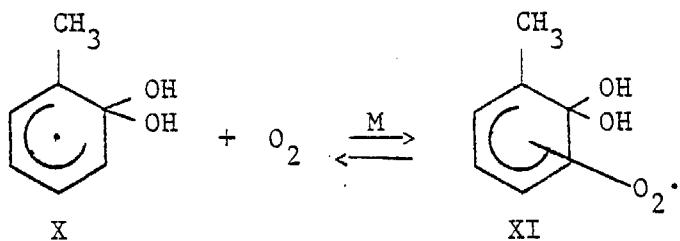
The major OH radical reaction pathway is in addition to the aromatic ring (Atkinson et al., 1979), and thermochemical calculations (Benson, 1976) show that radical X is the most thermochemically favorable adduct. Its formation is thus assumed to be the sole pathway.



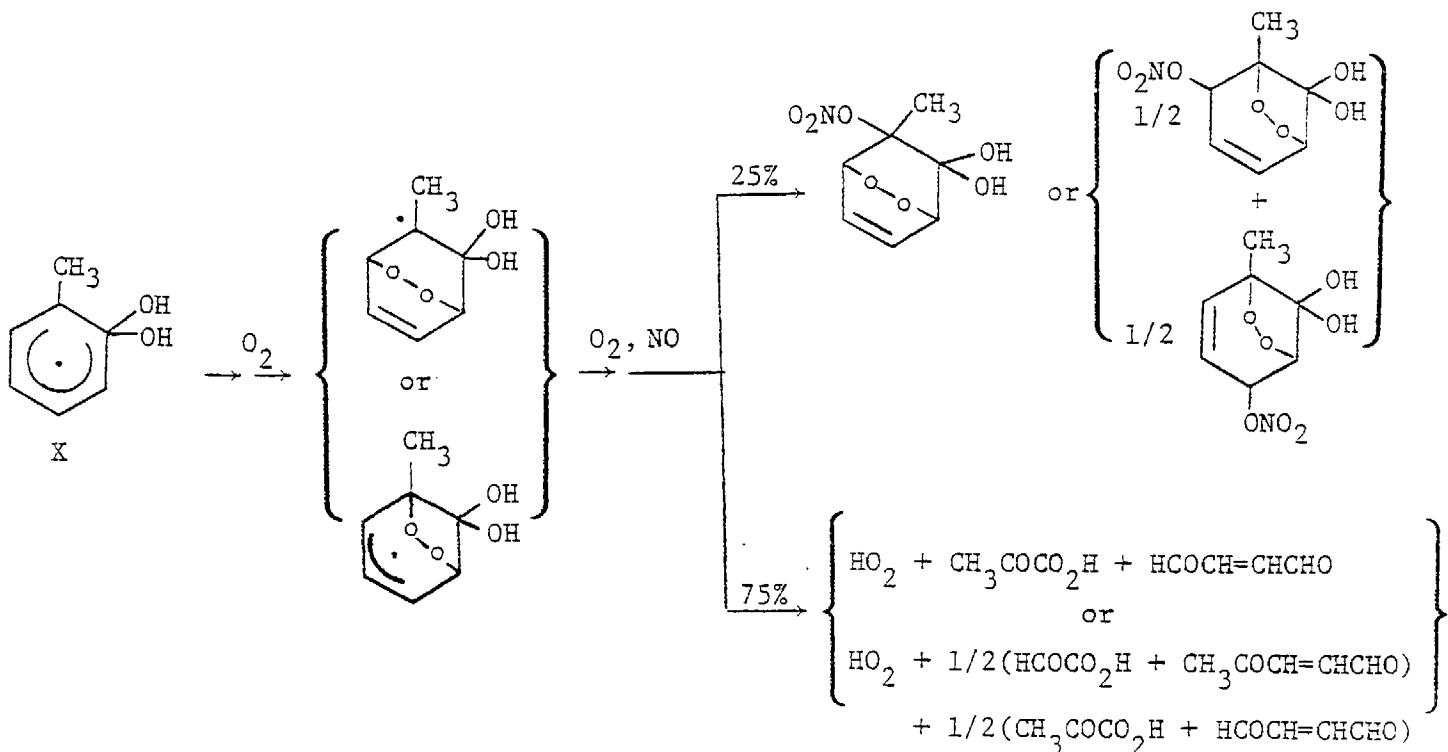
Species such as X can also react with NO<sub>2</sub> to give rise to the observed hydroxynitrotoluene isomers.



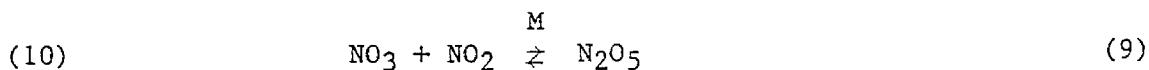
However, the dominant reaction of X is expected to be with O<sub>2</sub>:



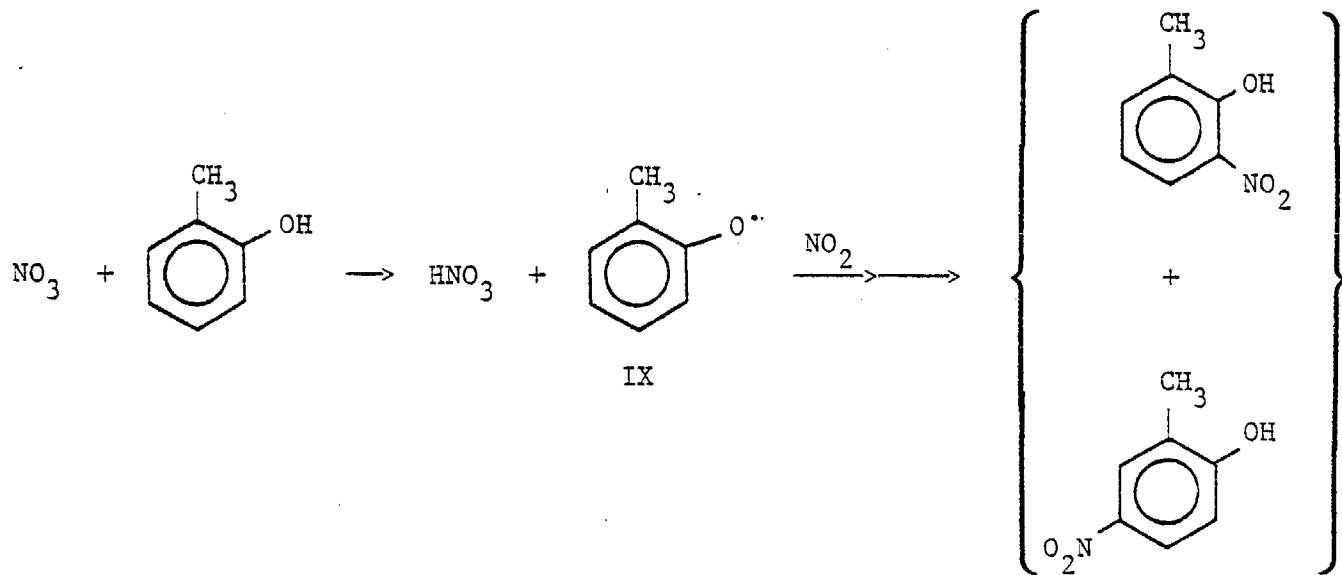
The subsequent reactions of radicals XI are assumed to be analogous to those of radical II formed in the toluene system. The various possible detailed reactions for these species are listed in Appendix B (substituent 1 = OH, 2 = CH<sub>3</sub> for the 1 adduct; substituent 1 = OH, 6 = CH<sub>3</sub> for the 3 adduct), and the overall processes are given in Appendix A as reactions 70-77. The best fit models predict that the major overall processes are as shown below:



There is evidence that there is an additional significant loss process for cresols in NO<sub>x</sub>-air systems. It has been independently observed by O'Brien (1979) and in our laboratories (Carter et al., 1980) that although the cresols do not react at significant rates with either O<sub>3</sub> (Atkinson et al., 1978b; Hendry, 1979; O'Brien, 1979) or NO<sub>2</sub> (O'Brien, 1979; Carter et al., 1980), they do appear to rapidly disappear in chambers dosed with NO<sub>2</sub> and O<sub>3</sub> together. Since O<sub>3</sub> and NO<sub>2</sub> react rapidly to form NO<sub>3</sub> and N<sub>2</sub>O<sub>5</sub> (Graham and Johnston, 1978)



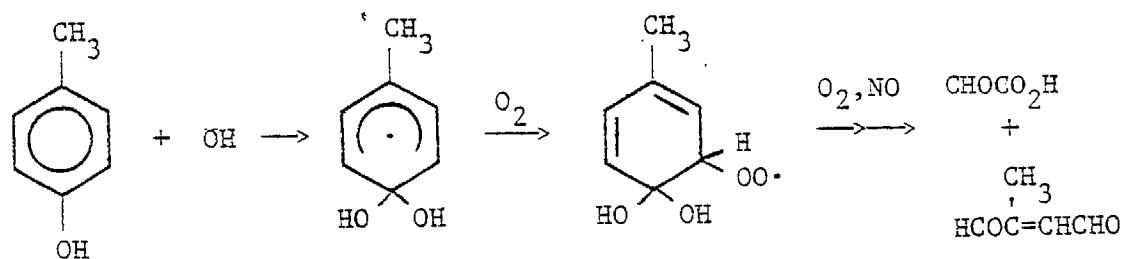
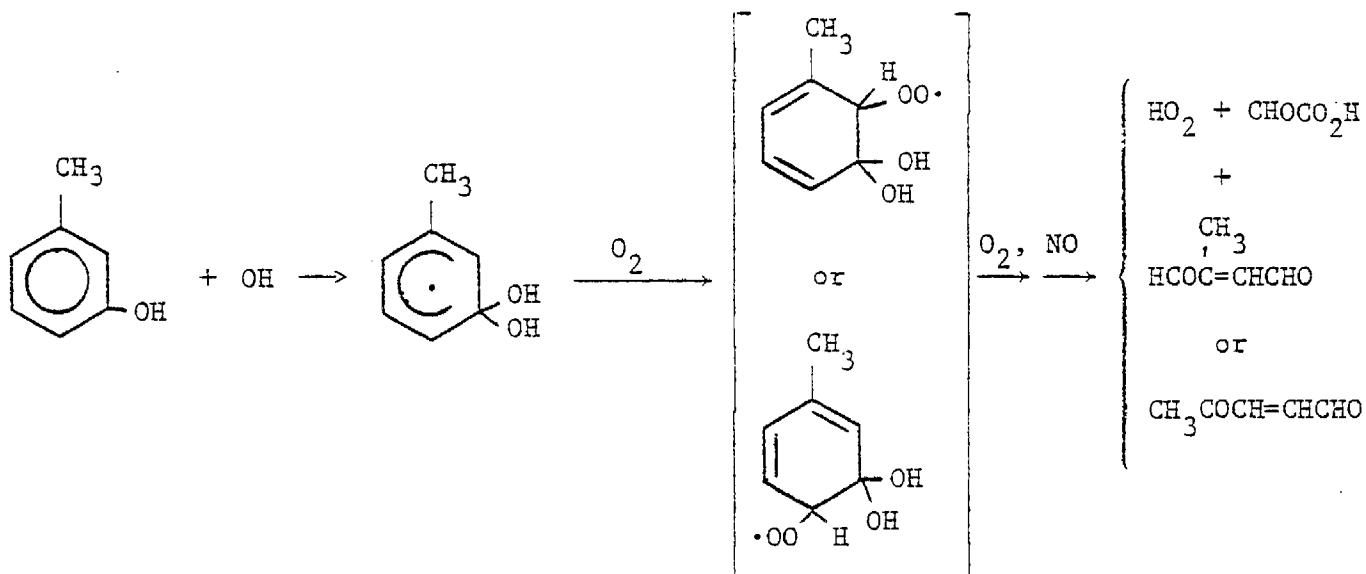
these observations can be attributed to rapid reaction of cresols with either  $\text{NO}_3$  or  $\text{N}_2\text{O}_5$ . Since  $\text{NO}_3$  is known to react with alkenes (Japar and Niki, 1975), it is probable that it is also  $\text{NO}_3$  which is reacting with the cresols. We have recently obtained, using a relative rate technique, a rate constant for the reaction of  $\text{NO}_3$  radicals with o-cresol of  $\sim 1.5 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ sec}^{-1}$  (Carter et al., 1980). As can be seen in Figure 43, this rate constant is sufficiently high that reaction with  $\text{NO}_3$  becomes a significant sink for o-cresol after  $\text{O}_3$  formation begins, and accounts for the rapid decrease in the o-cresol concentrations observed after their initial rise in the toluene- $\text{NO}_x$ -air runs. The observation that  $\text{NO}_3$  radicals react rapidly with phenol and the cresols, but only very slowly with toluene and methoxybenzene indicates that the reaction with phenol and the cresols proceeds via H atom abstraction from the substituent-OH group to form radical IX (Carter et al., 1980):



Hence this reaction is another explanation for the formation of the hydroxy-nitrotoluene isomers observed.

As noted previously, the order of the overall reactivity of the cresol isomers in  $\text{NO}_x$ -air systems is meta >> para > ortho (see Figure 36). This effect is larger than can be attributed to the relatively small differences in the OH + cresol rate constants (Atkinson et al., 1979; Atkinson et al., 1978b) (meta/ortho = 1.4; para/ortho = 1.1), but it can

readily be rationalized in terms of the mechanism. On the basis of the mechanisms which best fit the toluene- $\text{NO}_x$  and the o-cresol- $\text{NO}_x$  data, m- and p-cresol are expected to react as shown:



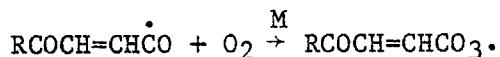
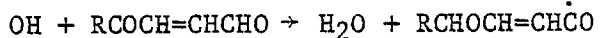
$\text{CHOCO}_2\text{H}$  formed in the m- and p-cresol systems is expected to be more reactive towards OH radicals than the  $\text{CH}_3\text{COCO}_2\text{H}$  formed in the o-cresol system, since it has the labile -CHO group. In addition, both 2-methyl-2-butene-1,4-dial and 2-pentene-1,4-dial are expected to give rise to methyl-glyoxal, a powerful photoinitiator, in their photooxidation mechanism (see Appendix A, reactions 100-141), which is not formed from the 2-butene-1,4-dial predicted in the o-cresol mechanism (the latter instead forming glyoxal, which is believed to have far lower quantum yields for photodecomposition (see Note 29, Appendix A)). Furthermore, in the m-cresol system, the OH radical may add to a significant extent at the 2-position, since the radical formed is stabilized by both the OH and the - $\text{CH}_3$  groups,

unlike analogous adducts for the other cresol isomers. Applying our mechanism this adduct is expected to give rise to methylglyoxal directly, which may explain the far greater reactivity of m-cresol relative to the o- and p-isomers.

Subsequent Reactions of Ring-Opening Products. The subsequent reactions of the ring cleavage products formed in the toluene and the cresol photooxidations are given in Appendix A. In many cases the mechanisms are uncertain and rate constants have had to be estimated; these are discussed in the associated notes. The following points concerning the reactions of these products should be noted:

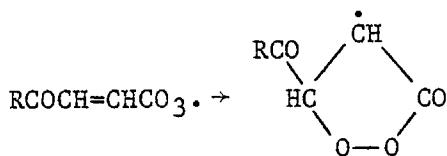
a) In order for the model to fit the smog chamber data, it must include the formation of radical initiator(s) in the toluene photooxidation mechanism which are not formed in the o-cresol system. The major initiator appears to be methylglyoxal, whose photolysis is also primarily responsible for the observed production of PAN, HCHO, and CH<sub>3</sub>ONO<sub>2</sub>. No other product predicted by our mechanism is believed to photodecompose to give radicals as rapidly as methylglyoxal (see Notes 20, 29 and 33 in Appendix A for brief discussions of benzaldehyde, glyoxal, and conjugated γ-dicarbonyl photolyses, respectively).

b) There is a significant uncertainty in the photooxidation mechanism of the conjugated γ-dicarbonyls which are predicted to be formed as major products. These products are expected to react predominately with OH radicals, giving rise to unsaturated α-carbonyl peroxy radicals



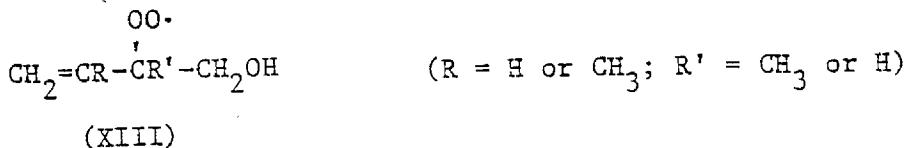
(XII)

These radicals could react with NO and NO<sub>2</sub> (e.g., reactions 110-113), in a manner analogous to the reactions of acyl peroxy radicals, forming unsaturated PAN analogues such as HCOCH=CHCO<sub>3</sub>NO<sub>2</sub>. However, these unsaturated peroxy radicals may also undergo cyclization,



(XII)

resulting in the ultimate formation of glyoxal ( $R=H$ ) or PAN + methylglyoxal ( $R=CH_3$ ) (see Appendix A). It is not known at the present time whether this cyclization is rapid enough to compete with reaction of (XII) with NO or  $NO_2$ . The recent observation of methylvinylketone and methacrolein formation during the early stages (before significant ozone formation) of the  $NO_x$  photooxidation of isoprene (Arnts and Gay, 1979) indicates that in the case of the unsaturated alkyl peroxy radicals, (XIII) cyclization is negligible compared to reaction with NO.



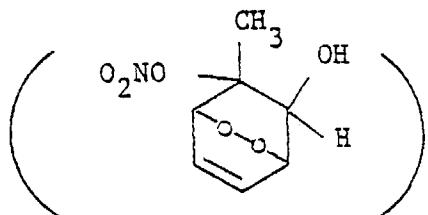
However, it is not clear that the unsaturated acylperoxy radicals such as (XII) formed in this system will react analogously, and hence it is necessary to consider both mechanistic options.

As can be seen in Figures 37 and 38, where results of the calculations assuming cyclization of (XII) is rapid, are compared with those assuming it is negligible, (compare Model A with B, C with D, or E with F) the uncertainty concerning the rate of this cyclization has a significant impact on model predictions concerning both the toluene and the cresol systems. It is this uncertainty which does not allow us to distinguish unambiguously whether these data are best fit by assuming [2.2.2] cyclization and predominant 3-addition of  $O_2$  to the OH-aromatic adduct (calculations A), or by assuming [3.2.1] cyclization dominates (calculations F), since the former assumes that cyclization of XII is negligible while the latter assumes it dominates. If the rate of this cyclization were known, one of these mechanisms could probably be eliminated.

Conclusions. The chemical kinetic computer models for irradiated toluene-benzaldehyde-o-cresol- $NO_x$ -air mixtures, which are discussed above and are consistent with available basic kinetic and mechanistic data and with reasonable thermochemical and kinetic estimates, have been shown to be capable of giving predictions of reactant and major and minor product concentration-time profiles which are in reasonably good agreement with results of well-characterized smog chamber irradiations performed with a variety of initial reactant concentrations. However, with the

information available to date, it is not possible to choose between various optional sets of equally reasonable reaction sequences. For example, the experimental data appear to be reasonably well fit by the two sets of mechanistic options discussed above. In addition, in our initial studies it was found that most of the concentration-time profiles, except for those of o-cresol, could be equally well fit by a model giving the same products as A, but assuming that organic nitrate formation from  $\text{RO}_2 + \text{NO}$  occurs ~40% of the time instead of ~25%, providing that fragmentation is increased by decreasing the formation of o-cresol from ~20% to ~8% of the overall reaction, and that the resulting increased production of PAN is compensated by changing the ratio  $k(\text{CH}_3\text{CO}_3 + \text{NO})/k(\text{CH}_3\text{CO}_3 + \text{NO}_2)$  from 1.5 to 2.0, which is within its range of uncertainty (Carter et al., 1979).

These chemical kinetic models predict the formation of products and reactive intermediates in aromatic- $\text{NO}_x$ -air photooxidations which have not yet been detected in such systems, and whose atmospheric chemistry is at best poorly characterized. Such products predicted in the toluene system include the  $\alpha$ -dicarbonyls glyoxal and methylglyoxal, and the  $\gamma$ -unsaturated dicarbonyls  $\text{RCOCH=CHCHO}$  ( $\text{R}=\text{H, CH}_3$ ) and possibly the corresponding peroxyacetyl nitrates  $\text{RCOCH=CHCO}_3\text{NO}_2$ , together with the alicyclic nitrate which is proposed to be formed from the OH-toluene- $\text{O}_2$  adduct and NO; for example



Furthermore, quantitative rate and mechanistic information is required for: the photolysis of benzaldehyde and the  $\alpha$ -carbonyl carboxylic acids, the fraction of the alkyl nitrate from the peroxy radical intermediates in the aromatic photooxidation mechanism, and the general atmospheric chemistry of  $\alpha$ -dicarbonyls and  $\gamma$ -unsaturated dicarbonyls.

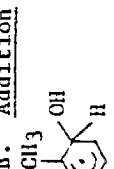
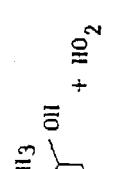
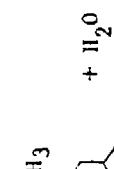
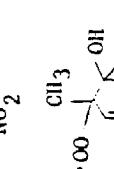
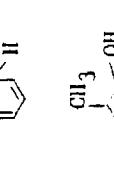
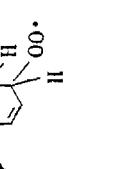
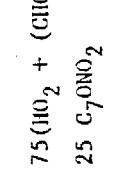
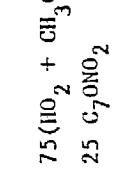
**APPENDIX A. Reactions and Rate Constants Used in the  $\text{NO}_x$ -Toluene-Air Model**

	Reaction	Rate constant cm molecule sec units <sup>a,b</sup>	Notes	References
<b>I. Inorganic Reactions</b>				
1	$\text{NO}_2 + \text{hv} \rightarrow \text{NO} + \text{O}(^3\text{P})$	$6.6 \times 10^{-3}$	1	Hampson & Garvin (1978)
2	$\text{O}(^3\text{P}) + \text{O}_2 + \text{M} \rightarrow \text{O}_3 + \text{M}$	$5.7 \times 10^{-34}$		Hampson & Garvin (1978)
3	$\text{O}(^3\text{P}) + \text{NO}_2 \rightarrow \text{NO} + \text{O}_2$	$9.1 \times 10^{-12}$		Hampson & Garvin (1978)
4	$\text{O}_3 + \text{NO} \rightarrow \text{NO}_2 + \text{O}_2$	$1.8 \times 10^{-14}$		Hampson & Garvin (1978)
5	$\text{O}_3 + \text{NO}_2 \rightarrow \text{NO}_3 + \text{O}_2$	$3.7 \times 10^{-17}$		Hampson & Garvin (1978)
6	$\text{NO} + \text{NO}_3 \rightarrow 2\text{NO}_2$	$1.9 \times 10^{-11}$		Graham & Johnston (1978)
7	$\text{NO}_2 + \text{NO}_3 \rightarrow \text{NO} + \text{NO}_2 + \text{O}_2$	$4.3 \times 10^{-16}$		Graham & Johnston (1978)
8	$\text{NO} + \text{NO} + \text{O}_2 \rightarrow 2\text{NO}_2$	$1.9 \times 10^{-38}$		Hampson & Garvin (1978)
9	$\text{NO}_2 + \text{NO}_3 \rightarrow \text{N}_2\text{O}_5$	$1.9 \times 10^{-12}$	2	Graham & Johnston (1978)
10	$\text{N}_2\text{O}_5 \rightarrow \text{NO}_2 + \text{NO}_3$	$0.15$	2,3	Connell & Johnston (1979)
11	$\text{N}_2\text{O}_5 + \text{H}_2\text{O} \rightarrow 2\text{HNO}_3$	$3 \times 10^{-21}$	Estimated 4,5	
12	$\text{NO}_3 + \text{hv} \rightarrow \text{NO} + \text{O}_2$	$2.8 \times 10^{-2}$	1	Graham & Johnston (1978)
13	$\text{NO}_3 + \text{hv} \rightarrow \text{NO}_2 + \text{O}(^3\text{P})$	$7.4 \times 10^{-2}$	1	Graham & Johnston (1978)
14	$\text{O}_3 + \text{hv} \rightarrow \text{O}_2 + \text{O}(^3\text{P})$	$(2.4 \times 10^{-4})$	1	Hampson & Garvin (1978)
15	$\text{O}_3 + \text{hv} \rightarrow \text{O}_2 + \text{O}(^1\text{D})$	$9.8 \times 10^{-6}$	1	Hampson & Garvin (1978)
16	$\text{O}(^1\text{D}) + \text{M} \rightarrow \text{O}(^3\text{P}) + \text{M}$	$3.0 \times 10^{-11}$		Streit et al. (1976)
17	$\text{O}(^1\text{D}) + \text{H}_2\text{O} \rightarrow 2\text{OH}$	$2.3 \times 10^{-10}$		Hampson & Garvin (1978)
18	$\text{OH} + \text{NO} \rightarrow \text{HONO}$	$6.8 \times 10^{-12}$	2	Anastasi & Smith (1978) Overend et al. (1976)
19	$\text{OH} + \text{NO}_2 \rightarrow \text{HNO}_3$	$1.1 \times 10^{-11}$	2	Hampson & Garvin (1978)
20	$\text{HONO} + \text{hv} \rightarrow \text{OH} + \text{NO}$	$1.1 \times 10^{-3}$	1	Stockwell & Galvert (1978)
21	$\text{OH} + \text{O}_3 \rightarrow \text{HO}_2 + \text{O}_2$	$8.5 \times 10^{-14}$		Ravishankara et al. (1979)

APPENDIX A (cont.)

	Reaction	Rate constant cm molecule sec units <sup>a,b</sup>	Notes	References
22	$\text{HO}_2 + \text{O}_3 \rightarrow \text{OH} + 2\text{O}_2$	$2.1 \times 10^{-15}$		Zahniser & Howard (1978)
23	$\text{HO}_2 + \text{NO} \rightarrow \text{OH} + \text{NO}_2$	$8.1 \times 10^{-12}$		Howard & Evenson (1977)
24	$\text{HO}_2 + \text{NO}_2 \rightarrow \text{HO}_2\text{NO}_2$	$1.2 \times 10^{-12}$		Hampson & Garvin (1978)
25	$\text{HO}_2\text{NO}_2 \rightarrow \text{HO}_2 + \text{NO}_2$	0.15		Graham et al. (1977)
26	$\text{HO}_2 + \text{NO}_3 \rightarrow \text{HNO}_3 + \text{O}_2$	$3 \times 10^{-12}$	Estimated 6	Graham et al. (1977)
27	$\text{HO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + \text{O}_2$	$2.5 \times 10^{-12}$		Hampson & Garvin (1978)
28	$\text{HO}_2 + \text{HO}_2 + \text{H}_2\text{O} \rightarrow \text{H}_2\text{O}_2 + \text{O}_2 + \text{H}_2\text{O}$	$6.5 \times 10^{-30}$		Hamilton & Li (1977)
29	$\text{H}_2\text{O}_2 + h\nu \rightarrow 2\text{OH}$	$4.7 \times 10^{-6}$	7	Hamilton & Li (1977)
30	$\text{OH} + \text{CO} \rightarrow \text{CO}_2 + \text{H}$	$3.0 \times 10^{-13}$	1	
31	$\text{H} + \text{O}_2 + \text{M} \rightarrow \text{HO}_2 + \text{M}$	Fast		Hampson & Garvin (1978)
32	$\text{O}_3 \xrightarrow{\text{wall}}$	$2.8 \times 10^{-5}$	5	Pitts et al. (1977)
33	$\text{H}_2\text{O}_2 \xrightarrow{\text{wall}}$	$7.0 \times 10^{-5}$	5	Pitts et al. (1977)
34	$\gamma + h\nu \longrightarrow \text{OH}$	$(6-24) \times 10^7$	5,8	Carter et al. (1979)
	<u>III. Toluene Photooxidation Reactions</u>			
	A. Abstraction			
35	$\text{OH} + \text{toluene} \rightarrow \text{C}_6\text{H}_5\dot{\text{C}}\text{H}_2 + \text{H}_2\text{O}$	$1.0 \times 10^{-12}$		Perry et al. (1977a) Kenley et al. (1978)
36	$\text{C}_6\text{H}_5\dot{\text{C}}\text{H}_2 + \text{O}_2 \rightarrow \text{C}_6\text{H}_5\text{CH}_2\dot{\text{O}}_2$	Fast		
37	$\text{C}_6\text{H}_5\text{CH}_2\dot{\text{O}}_2 + \text{NO} \rightarrow \text{C}_6\text{H}_5\text{CH}_2\dot{\text{O}} + \text{NO}_2$	$6 \times 10^{-12}$		
38	$\text{C}_6\text{H}_5\text{CH}_2\dot{\text{O}}_2 + \text{NO} \rightarrow \text{C}_6\text{H}_5\text{CH}_2\text{ONO}_2$	$2 \times 10^{-12}$		
39	$\text{C}_6\text{H}_5\text{CH}_2\dot{\text{O}} + \text{O}_2 \rightarrow \text{C}_6\text{H}_5\text{CHO} + \text{HO}_2$	$1.2 \times 10^{-15}$		
40	$\text{C}_6\text{H}_5\text{CH}_2\dot{\text{O}} + \text{NO}_2 \rightarrow \text{C}_6\text{H}_5\text{ONO}_2$	$1.6 \times 10^{-11}$		

APPENDIX A (cont.)

	Reaction	Rate constant cm molecule sec units <sup>a,b</sup>	Notes	References
	B. Addition			
41	OH + toluene $\rightarrow$ 	$5.4 \times 10^{-12}$	10	Perry et al. (1977a) Kenley et al. (1978)
42	 + O <sub>2</sub> $\rightarrow$  + NO <sub>2</sub>	$1.2 \times 10^{-15}$	11	
43	 + NO <sub>2</sub> $\rightarrow$  + H <sub>2</sub> O	$5.2 \times 10^{-12}$	12	Kenley et al. (1978)
44	 + O <sub>2</sub> $\xrightarrow{M}$ 	(Slow) $3.5 \times 10^{-15}$ Mech. A, B only		
45	 + O <sub>2</sub> $\xrightarrow{M}$ 	(Slow) $3.5 \times 10^{-15}$ Mech. C, D (adjusted) $2,13$		
46 <sup>c</sup>	 NO $\xrightarrow{O_2}$ 0.75(NO <sub>2</sub> ) <sub>2</sub> + (CHO) <sub>2</sub> + CH <sub>3</sub> COCl=CHClO + 0.25 C <sub>7</sub> ONO <sub>2</sub>	(Slow) Fast	Mech. A, B, E-II Mech. C, D	14,15
47 <sup>c</sup>	NO $\xrightarrow{O_2}$ 0.75(NO <sub>2</sub> ) <sub>2</sub> + CH <sub>3</sub> COCHO + HCOCl=CHClO + NO <sub>2</sub> + 0.25 C <sub>7</sub> ONO <sub>2</sub>	Fast (Slow)	Mech. A, B Mech. C-II	15,16

## APPENDIX A (cont.)

	Reaction	Rate constant cm molecule <sup>-1</sup> sec <sup>-1</sup> units <sup>a,b</sup>	Notes	References
48 <sup>c</sup>	<p> <math>\xrightarrow{\text{NO}_2, \text{O}_2}</math> 0.75(HIO<sub>2</sub> + 1/2(ClO)<sub>2</sub> + 1/2CH<sub>3</sub>COCIO          + 1/2HCOCH=CHCHO + 1/2CH<sub>3</sub>COC(=CHCHO + NO<sub>2</sub>)          + 0.25C<sub>7</sub>ONO<sub>2</sub> </p>	$\left\{ \begin{array}{l} \text{(Slow)} \\ \text{Fast} \end{array} \right.$	Mech. A-E, G, H Mech. E, F	14, 17
49 <sup>c</sup>	<p> <math>\xrightarrow{\text{NO}_2, \text{O}_2}</math> 0.75(HIO<sub>2</sub> + 1/2(ClO)<sub>2</sub> + 1/2CH<sub>3</sub>COCIO          + 1/2HCOCH=CHCHO + 1/2CH<sub>3</sub>COC(=CHCHO + NO<sub>2</sub>)          + 0.25C<sub>7</sub>ONO<sub>2</sub> </p>	$\left\{ \begin{array}{l} \text{(Slow)} \\ \text{Fast} \end{array} \right.$	Mech. A-E, G, H Mech. E, F	16, 17
50 <sup>c</sup>	<p> <math>\xrightarrow{\text{NO}_2, \text{O}_2}</math> 0.75(HIO + (ClO)<sub>2</sub> + CH<sub>3</sub>COC(=CHCHO + NO<sub>2</sub>)          + 0.25C<sub>7</sub>ONO<sub>2</sub> </p>	$\left\{ \begin{array}{l} \text{(Slow)} \\ \text{Fast} \end{array} \right.$	Mech. A-F, H Mech. G	14, 18
51 <sup>c</sup>	<p> <math>\xrightarrow{\text{NO}_2, \text{O}_2}</math> 0.75(HIO + (ClO)<sub>2</sub> + CH<sub>3</sub>COC(=CHCHO + NO<sub>2</sub>)          + 0.25C<sub>7</sub>ONO<sub>2</sub> </p>	$\left\{ \begin{array}{l} \text{(Slow)} \\ \text{Fast} \end{array} \right.$	Mech. A-F, H Mech. G	16, 18
52 <sup>c</sup>	<p> <math>\xrightarrow{\text{NO}_2, \text{O}_2}</math> 0.75(HIO<sub>2</sub> + 2(ClO)<sub>2</sub> + CH<sub>3</sub>COCIO + NO<sub>2</sub>)          + 0.25C<sub>7</sub>ONO<sub>2</sub> </p>	$\left\{ \begin{array}{l} \text{(Slow)} \\ \text{Fast} \end{array} \right.$	Mech. A-G Mech. H	14, 19

	Reaction	Rate constant cm molecule sec units <sup>a,b</sup>	Notes	References
53 <sup>c</sup>	$\text{Cl}_3\text{C}(\text{OH})\text{C}_6\text{H}_4\text{OO} \xrightarrow{\text{NO}_2, \text{O}_2} 0.75(\text{HO}_2 + 2(\text{CHO})_2 + \text{Cl}_3\text{COCHO} + \text{NO}_2)$	$\left\{ \begin{array}{l} (\text{Slow}) \\ \text{Fast} \end{array} \right.$ $\left\{ \begin{array}{l} \text{Mech. A-G} \\ \text{Mech. II} \end{array} \right.$	14, 19	
III. Organic Product Photooxidations				
A. Benzaldehyde				
54	$\text{OH} + \text{C}_6\text{H}_5\text{CHO} \rightarrow \text{H}_2\text{O} + \text{C}_6\text{H}_5\text{CO}$	$1.3 \times 10^{-11}$		$\left\{ \begin{array}{l} \text{Niki et al. (1978)} \\ \text{Atkinson et al. (1979)} \end{array} \right.$
55	$\text{C}_6\text{H}_5\text{CHO} + \text{hv} \rightarrow \text{Products}$	$3 \times 10^{-5}$	Adjusted	20
56	$\text{C}_6\text{H}_5\dot{\text{CO}} + \text{O}_2 \rightarrow \text{C}_6\text{H}_5\dot{\text{CO}}_3$	Fast		
57	$\text{C}_6\text{H}_5\dot{\text{CO}}_3 + \text{NO}_2 \xrightarrow{\text{M}} \text{C}_6\text{H}_5\text{CO}_3\text{NO}_2$	$5 \times 10^{-12}$	21	
58	$\text{C}_6\text{H}_5\text{CO}_3\text{NO}_2 \rightarrow \text{C}_6\text{H}_5\dot{\text{CO}}_3 + \text{NO}_2$	$3.3 \times 10^{-4}$		Hendry & Kenley (1979)
59	$\text{C}_6\text{H}_5\dot{\text{CO}}_3 + \text{NO} \rightarrow \text{C}_6\text{H}_5\dot{\text{CO}}_2 + \text{NO}_2$	$8 \times 10^{-12}$		21
60	$\text{C}_6\text{H}_5\dot{\text{CO}}_2 \rightarrow \text{C}_6\text{H}_5\cdot + \text{CO}_2$	Fast	6	
61	$\text{C}_6\text{H}_5\cdot + \text{O}_2 \xrightarrow{\text{M}} \text{C}_6\text{H}_5\dot{\text{O}}$	Fast		
62	$\text{C}_6\text{H}_5\dot{\text{O}}_2 + \text{NO} \rightarrow \text{C}_6\text{H}_5\dot{\text{O}} + \text{NO}_2$	$6 \times 10^{-12}$	Ratio adjusted	9
63	$\text{C}_6\text{H}_5\dot{\text{O}}_2 + \text{NO} \xrightarrow{\text{M}} \text{C}_6\text{H}_5\text{ONO}_2$	$2 \times 10^{-12}$		

## APPENDIX A (cont.)

	Reaction	Rate constant cm molecule sec units <sup>a,b</sup>	Notes	References
64	$\text{C}_6\text{H}_5\text{O}^\cdot + \text{NO}_2 \xrightarrow{\text{M}} \text{C}_6\text{H}_5(\text{OH})\text{NO}_2$ (o- and p-)	$1.6 \times 10^{-11}$	6	Niki et al. (1979)
65	$\text{C}_6\text{H}_5\text{O}^\cdot + \text{HO}_2 \rightarrow \text{C}_6\text{H}_5\text{OH} + \text{O}_2$	$3 \times 10^{-12}$	22	
	B. <u>o-Cresol</u>			
66	$\text{OH} + \text{C}_6\text{H}_5\text{OH} \xrightarrow{\text{M}} \text{C}_6\text{H}_5\text{O}^\cdot + \text{H}_2\text{O}$	$4.7 \times 10^{-11}$	23	Atkinson et al. (1976b)
67	$\text{C}_6\text{H}_5\text{OH} + \text{NO}_2 \xrightarrow{\text{M}} \text{C}_6\text{H}_5\text{O}^\cdot + \text{H}_2\text{O} + \text{NO}_2$	$5.2 \times 10^{-12}$	24	
68	$\text{C}_6\text{H}_5\text{O}^\cdot + \text{O}_2 \xrightarrow{\text{M}} \text{C}_6\text{H}_5\text{OO}^\cdot + \text{H}_2\text{O}$	(Slow)	{ Mech. A, B only }	
69	$\text{C}_6\text{H}_5\text{O}^\cdot + \text{O}_2 \xrightarrow{\text{M}} \text{C}_6\text{H}_5\text{OOH} + \text{H}_2\text{O}$	$3.5 \times 10^{-15}$	{ Mech. C, D; (adjusted) }	2, 25
70 <sup>c</sup>	$\text{C}_6\text{H}_5\text{O}^\cdot + \text{NO}_2 \xrightarrow{\text{M}} \text{C}_6\text{H}_5\text{OOH} + \text{NO}_2$	$3.5 \times 10^{-15}$	{ Mech. A, B; (adjusted) }	
		(Slow)	{ Mech. C, D only }	
		Fast	Mech. C, D	15, 26

## APPENDIX A (cont.)

	Reaction	Rate constant cm molecule sec units <sup>a,b</sup>	Notes	References
71 <sup>c</sup>	 $\xrightarrow{\text{NO}, \text{O}_2}$ 0.75( $\text{HO}_2$ + $\text{HOOCCHO} + \text{CHCO=CHCHO} + \text{NO}_2$ )	{Fast (Slow)}	Mech. A,B Mech. C-H	15,27
72 <sup>c</sup>	 $\xrightarrow{\text{NO}, \text{O}_2}$ 0.75( $\text{HO}_2$ + 1/2 $\text{HOOCCHO} + 1/2 \text{HOOCOCCH}_3 + 1/2 \text{HOOCCHO} + 1/2 \text{CH}_3\text{COCH=CHCHO} + \text{NO}_2$ ) + 0.25 $\text{C}_7\text{ONO}_2$	{(Slow) Fast}	Mech. A-E,G,H Mech. E,F	17,26
73 <sup>c</sup>	 $\xrightarrow{\text{NO}, \text{O}_2}$ 0.75( $\text{HO}_2$ + 1/2 $\text{HOOCCHO} + 1/2 \text{HOOCOCCH}_3 + 1/2 \text{HOOCCHO} + 1/2 \text{CH}_3\text{COCH=CHCHO} + \text{NO}_2$ ) + 0.25 $\text{C}_7\text{ONO}_2$	{(Slow) Fast}	Mech. A-E,G,H Mech. E,F	17,27
74 <sup>c</sup>	 $\xrightarrow{\text{NO}, \text{O}_2}$ 0.75( $\text{HO}_2$ + $(\text{CHO})_2 + \text{CH}_3\text{CO}(\text{OH})_2\text{CHO} + \text{NO}_2$ ) + 0.25 $\text{C}_7\text{ONO}_2$	{(Slow) Fast}	Mech. A-F,H Mech. G	18,26
75 <sup>c</sup>	 $\xrightarrow{\text{NO}, \text{O}_2}$ 0.75( $\text{HO}_2$ + $(\text{CHO})_2 + \text{CH}_3\text{CO}(\text{OH})_2\text{CHO} + \text{NO}_2$ ) + 0.25 $\text{C}_7\text{ONO}_2$	{(Slow) Fast}	Mech. A-F,H Mech. G	18,27

APPENDIX A (cont.)

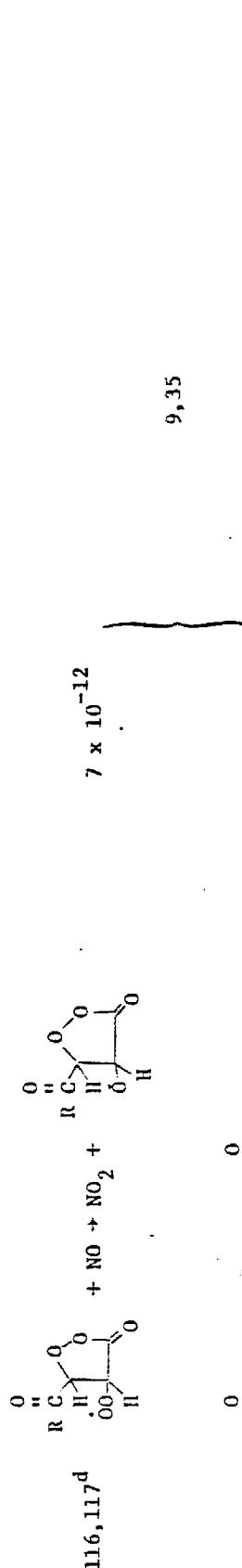
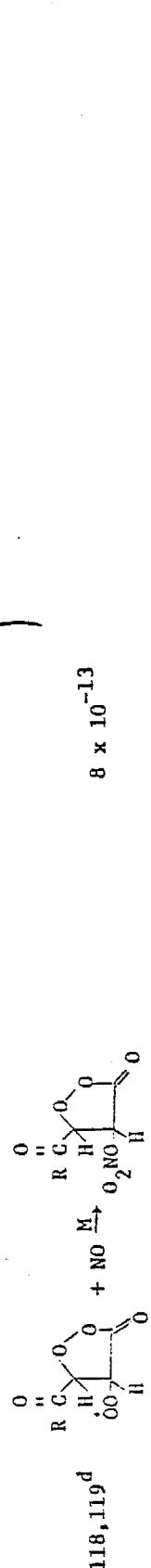
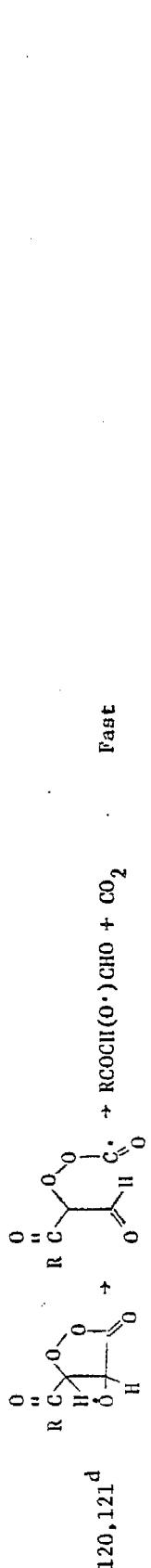
	Reaction	Rate constant cm molecule sec units <sup>a,b</sup>	Notes	References
76 <sup>c</sup>	$\text{OO} \begin{array}{c} \text{CH}_3 \\   \\ \text{C} \end{array} \begin{array}{c} \text{OH} \\   \\ \text{O} \end{array} \xrightarrow{\text{NO}, \text{O}_2} 0.75(\text{HO}_2 + 3/2(\text{CHO})_2 + 1/2\text{CH}_3\text{COCHO}$ $+ 1/2\text{HOCO CHO} + 1/2\text{HOCOCOCH}_3 + \text{NO}_2)$ $+ 0.25\text{C}_7\text{ONO}_2$	$\left\{ \begin{array}{l} (\text{Slow}) \\ \text{Fast} \end{array} \right.$ $\begin{array}{ll} \text{Mech. A-G} & \text{Mech. H} \end{array}$		19, 26
77 <sup>c</sup>	$\text{CH}_3 \begin{array}{c} \text{OH} \\   \\ \text{C} \end{array} \begin{array}{c} \text{OH} \\   \\ \text{O} \end{array} \xrightarrow{\text{NO}, \text{O}_2} 0.75(\text{HO}_2 + 3/2(\text{CHO})_2 + 1/2\text{CH}_3\text{COCHO}$ $+ 1/2\text{HOCOCHO} + 1/2\text{HOCOCOCH}_3 + \text{NO}_2)$ $+ 0.25\text{C}_7\text{ONO}_2$	$\left\{ \begin{array}{l} (\text{Slow}) \\ \text{Fast} \end{array} \right.$ $\begin{array}{ll} \text{Mech. A-G} & \text{Mech. H} \end{array}$		19, 27
78	$\text{NO}_3 + \text{CH}_3 \begin{array}{c} \text{OH} \\   \\ \text{C} \end{array} \rightarrow \text{CH}_3 \begin{array}{c} \text{O} \cdot \\   \\ \text{C} \end{array} + \text{HNO}_3$	$1.5 \times 10^{-11}$	28	Carter et al. (1979)
79	$\text{CH}_3 \begin{array}{c} \text{O} \cdot \\   \\ \text{C} \end{array} + \text{NO}_2 \xrightarrow{\text{M}} \text{CH}_3 \begin{array}{c} \text{O} \cdot \\   \\ \text{C} \end{array} \text{ONO}_2 \text{ or } \text{CH}_3 \begin{array}{c} \text{OH} \\   \\ \text{C} \end{array} \text{ONO}_2$	$1.6 \times 10^{-11}$	6	
80	G. Glyoxal	(Slow)		29
81	$(\text{CHO})_2 + \text{hv} \rightarrow \text{Products}$	$2 \times 10^{-11}$		30
82	$\text{HOCO} + \text{HO} \rightarrow \text{H}_2\text{O} + \text{HCO}\dot{\text{C}}$	Fast		

## APPENDIX A (cont.)

	Reaction	Rate constant cm molecule sec units <sup>a,b</sup>	Notes	References
<b>D. Methyl Glyoxal (And its Products)</b>				
83	HCO + O <sub>2</sub> → HO <sub>2</sub> + CO	5.6 × 10 <sup>-12</sup>		Washida et al. (1974) Shibuya et al. (1977)
84	CH <sub>3</sub> COClO + hν → CH <sub>3</sub> CO + HCO	1.0 × 10 <sup>-3</sup>	1,6	
85	OH + CH <sub>3</sub> COCOO → H <sub>2</sub> O + CH <sub>3</sub> COCO	1.6 × 10 <sup>-11</sup>	30	
86	CH <sub>3</sub> COCO → CH <sub>3</sub> CO + CO	Fast	6	
87	CH <sub>3</sub> CO + O <sub>2</sub> → CH <sub>3</sub> CO <sub>2</sub>	Fast	6	
88	CH <sub>3</sub> CO <sub>2</sub> + NO → CH <sub>3</sub> CO <sub>2</sub> + NO <sub>2</sub>	8 × 10 <sup>-12</sup>	21	
89	CH <sub>3</sub> CO <sub>2</sub> + NO <sub>2</sub> → CH <sub>3</sub> CO <sub>2</sub> NO <sub>2</sub>	5 × 10 <sup>-12</sup>	21	
90	CH <sub>3</sub> CO <sub>2</sub> NO <sub>2</sub> → CH <sub>3</sub> CO <sub>2</sub> + NO <sub>2</sub>	8.0 × 10 <sup>-4</sup>		Hendry & Kenley (1977) Cox & Roffey (1977)
91	CH <sub>3</sub> CO <sub>2</sub> → CH <sub>3</sub> • + CO <sub>2</sub>	Fast	6	
92	CH <sub>3</sub> • + O <sub>2</sub> → CH <sub>3</sub> OO <sub>2</sub>	Fast		
93	CH <sub>3</sub> OO <sub>2</sub> + NO → CH <sub>3</sub> • + NO <sub>2</sub>	8 × 10 <sup>-12</sup>	9	
94	CH <sub>3</sub> • + NO <sub>2</sub> → CH <sub>3</sub> ONO <sub>2</sub>	1.3 × 10 <sup>-11</sup>	6	
95	CH <sub>3</sub> • + NO <sub>2</sub> → HCHO + HONO	2.1 × 10 <sup>-12</sup>	6	

## APPENDIX A (cont.)

	Reaction	Rate constant cm molecule sec units <sup>a,b</sup>	Notes	References
96	$\text{CH}_3\dot{\text{O}} + \text{O}_2 \rightarrow \text{HCHO} + \text{HO}_2$	$1.2 \times 10^{-15}$		6
97	$\text{HCHO} + \text{hv} \rightarrow \text{H} + \text{HCO}$	$1.5 \times 10^{-5}$		1 Horowitz & Calvert (1978)
98	$\text{HCHO} + \text{hv} \rightarrow \text{H}_2 + \text{CO}$	$4.1 \times 10^{-5}$		
99	$\text{OH} + \text{HCHO} \rightarrow \text{H}_2\text{O} + \text{HCO}$	$9.4 \times 10^{-12}$		Atkinson & Pitts (1978)
	E. <u>Conjugated <math>\alpha</math>-Dicarbonyls</u>			
100	$\text{OH} + \text{HCHO}=\text{CHCHO} \rightarrow \text{H}_2\dot{\text{O}} + \text{HCOCH}=\text{CHCO}$	$3 \times 10^{-11}$		30,31
101	$\text{OH} + \text{CH}_3\text{COCH}=\text{CHCHO} + \text{H}_2\dot{\text{O}} + \text{CH}_3\text{COCH}=\text{CHCO}$	$1.6 \times 10^{-11}$		30,31
102,103 <sup>d</sup>	$\text{O}_3 + \text{RCOCH}=\text{CHCHO} \rightarrow \text{Products}$	(Slow)		32
104,105 <sup>d</sup>	$\text{RCOCH}=\text{CHCHO} + \text{hv} \rightarrow \text{Products}$	(Slow)		33
106,107 <sup>d</sup>	$\text{RCOCH}=\text{CHCO} + \text{O}_2 \xrightarrow{\text{M}} \text{RCOCH}=\text{CHCO}_3$	Fast		
		$\left. \begin{array}{l} (\text{Slow}) \\ \text{Fast} \end{array} \right\} \begin{array}{l} \text{Mech. A,G,E} \\ \text{Mech. B,D,F} \end{array}$		34
108,109 <sup>d</sup>	$\text{RCOCH}=\text{CHCO}_3 \rightarrow \text{R} \begin{array}{c} \text{O} \\    \\ \text{C} - \text{C} - \text{O} \\    \\ \text{O} \end{array} \text{O}$			
110,111 <sup>d</sup>	$\text{RCOCH}=\text{CHCO}_3 + \text{NO} \rightarrow \text{NO}_2 + \text{RCOCH}=\text{CHCO}_2$	$8 \times 10^{-12}$		21
112,113 <sup>d</sup>	$\text{RCOCH}=\text{CHCO}_3 + \text{NO}_2 \xrightarrow{\text{M}} \text{RCOCH}=\text{CHCO}_3\text{NO}_2$	$5 \times 10^{-12}$		21
114,115 <sup>d</sup>	$\text{R} \begin{array}{c} \text{O} \\    \\ \text{C} - \text{C} - \text{O} \\    \\ \text{O} \end{array} + \text{O}_2 \xrightarrow{\text{M}} \text{R} \begin{array}{c} \text{C} \\    \\ \text{C} - \text{C} - \text{O} \\    \\ \text{O} \end{array} \text{O} \text{O}$	Fast		

	Reaction	Rate constant cm molecule sec units <sup>a,b</sup>	Notes	References
116, 117 <sup>d</sup>		$7 \times 10^{-12}$		9, 35
118, 119 <sup>d</sup>		$8 \times 10^{-13}$		
120, 121 <sup>d</sup>		Fast		
122	$\text{HCOCH}(\text{O}^\cdot)\text{CHO} + \text{NO} + (\text{ClO})_2$	Fast		6
123	$\text{CH}_3\text{COCH}(\text{O}^\cdot)\text{CHO} + 1/2(\text{CH}_3\dot{\text{C}}\text{O} + (\text{ClO})_2)$ $+ 1/2 (\text{CH}_3\text{COCHO} + \text{NCO})$	Fast		6
124, 125 <sup>d</sup>	$\text{RCOCH}=\text{CHCO}_2^\cdot \rightarrow \text{RCOCH}=\dot{\text{C}}\text{H} + \text{CO}_2$	Fast		6
126, 127 <sup>d</sup>	$\text{RCOCH}=\dot{\text{C}}\text{H} + \text{O}_2 \xrightarrow{\text{M}} \text{RCOCH}=\text{CHO}^\cdot$	Fast		
128, 129 <sup>d</sup>	$\text{RCOCH}=\text{CHO}_2^\cdot + \text{NO} \rightarrow \text{NO}_2 + \text{RCOCH}=\text{CHO}^\cdot \leftrightarrow \text{RCO}\dot{\text{C}}\text{HO}$	$7 \times 10^{-12}$		9, 35
130, 131 <sup>d</sup>	$\text{RCOCH}=\text{CHO}_2^\cdot + \text{NO} \xrightarrow{\text{M}} \text{RCOCH}=\text{CHONO}_2$	$8 \times 10^{-13}$		
132, 133 <sup>d</sup>	$\text{RCO}\dot{\text{C}}\text{HO} + \text{O}_2 \xrightarrow{\text{M}} \text{RCOCH}(\text{O}_2^\cdot)\text{CHO}$	Fast		

## APPENDIX A (cont.)

	Reaction	Rate constant cm molecule sec units <sup>a,b</sup>	Notes	References
134,135 <sup>d</sup>	$\text{RCOCH(O}_2\cdot\text{)CHO} + \text{NO} \rightarrow \text{RCOCH(O}\cdot\text{)CHO} + \text{NO}_2$	$7 \times 10^{-12}$		9, 35
136,137 <sup>d</sup>	$\text{RCOCH(O}_2\cdot\text{)CHO} + \text{NO} \xrightarrow{\text{M}} \text{RCOCH(ONO}_2\text{)CHO}$	$8 \times 10^{-13}$		
138	$\text{HCOCH(O}\cdot\text{)CHO} \rightarrow (\text{CHO})_2 + \text{HCO}$	Fast		6
139	$\text{CH}_3\text{COCH(O}\cdot\text{)CHO} \rightarrow 1/2(\text{CH}_3\dot{\text{C}}\text{O} + (\text{CHO})_2)$ $+ 1/2(\text{HCO} + \text{CH}_3\text{COCCHO})$	Fast		6
140,141 <sup>d</sup>	$\text{RCOCH=CHCO}_3\text{NO}_2 \rightarrow \text{RCOCH=CHCO}_3 + \text{NO}_2$	$8.0 \times 10^{-4}$		36
	<u>F. <math>\beta</math>-Hydroxy-<math>\beta</math>-Dicarbonyls</u>			
142	$\text{CH}_3\text{COCH(OH)CHO} + \text{OH} \rightarrow \text{CH}_3\dot{\text{C}}\text{O}(\text{OH})\text{CHO} + \text{H}_2\text{O}$	$6 \times 10^{-12}$		37
143	$\text{CH}_3\dot{\text{C}}\text{O}(\text{OH})\text{CHO} + \text{O}_2 \rightarrow \text{NO}_2 + \text{CH}_3\text{COCOCNO}$	Fast		39
144	$\text{CH}_3\text{COCOCHO} \rightarrow \text{CH}_3\text{COCO} + \text{CO}$	Fast		
145,146 <sup>e</sup>	$\text{CH}_3\text{COCX(OH)CHO} + \text{OH} \rightarrow \text{CH}_3\text{COCX(OH)}\dot{\text{C}}\text{O}$ $\text{CH}_3\text{COCX(OH)}\dot{\text{C}}\text{O} + \text{O}_2 \xrightarrow{\text{M}} \text{CH}_3\text{COCX(OH)}\dot{\text{C}}\text{O}_2$	$1.6 \times 10^{-11}$		30
147,148 <sup>e</sup>	$\text{CH}_3\text{COCX(OH)}\dot{\text{C}}\text{O} + \text{O}_2 \xrightarrow{\text{M}} \text{CH}_3\text{COCX(OH)}\dot{\text{C}}\text{O}_2$	Fast		
149,150 <sup>e</sup>	$\text{CH}_3\text{COCX(OH)}\dot{\text{C}}\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{COCX(OH)}\dot{\text{C}}\text{O}_2$	$8 \times 10^{-12}$		21
151,152 <sup>e</sup>	$\text{CH}_3\text{COCX(OH)}\dot{\text{C}}\text{O}_2 + \text{NO}_2 \rightarrow \text{CH}_3\text{COCX(OH)}\dot{\text{C}}\text{O}_2\text{NO}_2$	$5 \times 10^{-12}$		21
153,154 <sup>e</sup>	$\text{CH}_3\text{COCX(OH)}\dot{\text{C}}\text{O}_2 \rightarrow \text{CH}_3\text{COCX(OH)}\dot{\text{C}}\text{O}_2 + \text{CO}_2$	Fast		6
155,156 <sup>e</sup>	$\text{CH}_3\text{COCX(OH)}\dot{\text{C}}\text{O}_2 + \text{O}_2 \rightarrow \text{HO}_2 + \text{CH}_3\text{COCOX}$	Fast		38
157,158 <sup>e</sup>	$\text{CH}_3\text{COCX(OH)}\dot{\text{C}}\text{O}_2 \rightarrow \text{CH}_3\text{COCX(OH)}\dot{\text{C}}\text{O}_2 + \text{NO}_2$	$8.0 \times 10^{-4}$		36

## APPENDIX A (cont.)

Reaction	Rate constant cm <sup>3</sup> molecule sec units <sup>a,b</sup>	Notes	References
<b>G. <math>\alpha</math>-Carbonyl Acids</b>			
159 HOOCCHO + OH $\rightarrow$ HOOC $\dot{C}O$ + H <sub>2</sub> O	1.6 $\times$ 10 <sup>-11</sup>		30
160 HOOC $\dot{C}O$ + HO $\dot{C}O$ + CO		Fast	
161 HO $\dot{C}O$ + O <sub>2</sub> $\rightarrow$ HO <sub>2</sub> + CO <sub>2</sub>		Fast	
162, 163 <sup>d</sup> HOOCOCOR + hν $\rightarrow$ Products		(Slow)	39
164  + OH $\rightarrow$ Products + HO <sub>2</sub>	$\sim$ 6 $\times$ 10 <sup>-12</sup>		40
<b>IV. Hydroperoxides</b>			
165 RO <sub>2</sub> <sup>f</sup> + HO <sub>2</sub> $\rightarrow$ RO <sub>2</sub> H + O <sub>2</sub>	3 $\times$ 10 <sup>-12</sup>		6
166 RO <sub>2</sub> H <sup>f</sup> + hν $\rightarrow$ OH + HO <sub>2</sub> + Products	5 $\times$ 10 <sup>-6</sup>		6

<sup>a</sup> Rate constants are given for the conditions of the smog chamber runs listed in Table 1 (303 K, 735 torr, M=air). Photolysis rate constants are given for the light intensity and spectral distributions associated with runs 327-340 (Pitts et al., 1979b); photolysis rates for runs 266-281 are somewhat lower.

<sup>b</sup> First order reaction; sec<sup>-1</sup>; 2nd order reaction: cm<sup>3</sup> molecule<sup>-1</sup> sec<sup>-1</sup>; 3rd order reaction: cm<sup>6</sup> molecule<sup>-2</sup> sec<sup>-1</sup>. Zero order reaction (reaction 34 only) molecule cm<sup>3</sup> sec<sup>-1</sup>. "Fast" means that the reaction is the sole pathway for that particular species; the predictions are insensitive for the actual rate constant. "(Slow)", or rate constants given in parentheses mean that the reaction is assumed to be negligible or that the reaction has a negligible effect on the predictions of the model for the concentration regimes studied here.

<sup>c</sup> The reaction as written represents an overall process for which the detailed reactions involved are given in Appendix B.

<sup>d</sup> Reaction numbers refer to R = -H or -CH<sub>3</sub>, respectively.

<sup>e</sup> Reaction numbers refer to X = -H or X = -OH, respectively.

<sup>f</sup>"RO" refers to all radicals of the form RO<sub>2</sub> or RC<sub>3</sub> in the mechanism. RO<sub>2</sub>H is treated as a single species.

Notes

1.  $k_1$  was determined from the photolysis of  $\text{NO}_2$  in  $\text{N}_2$  (Pitts et al., 1979b; Darnall et al., 1979; Holmes et al., 1973). All other photolysis rate constants were derived as described previously (Carter et al., 1979) from the absorption coefficients of the photolyzing species, the quantum yields, and the relative spectral distribution of the photolysis light (Pitts et al., 1979b).
2. The rate constant is pressure dependent and is given for 1 atmosphere of air.
3.  $k_9$  was derived from the equilibrium constant of Graham and Johnston (1978) combined with the  $\text{N}_2\text{O}_5$  decomposition rate constant,  $k_{10}$ , derived by interpolating the data of Connell and Johnston (1979), which was reported at various  $\text{N}_2$  number densities, to 760 torr of  $\text{N}_2$ .
4. Value consistent with that required for the  $\text{NO}_x$ -n-butane-propene-air system (Carter et al., 1979), and is also consistent with the gas phase upper limit of  $k_{11} \leq 1.3 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ sec}^{-1}$  obtained by Morris and Niki (1973).
5. Value given is specific for the SAPRC evacuable chamber.
6. Based on the assignment or estimate of Carter et al. (1979) for the same or for analogous reactions.
7. Pseudo-third order reaction added to account for the observed effects of humidity on this reaction (Hamilton and Lii, 1977).  $k_{28}$  was calculated to be consistent with the data of Hamilton and Lii (1977) and the  $\text{HO}_2\cdot\text{H}_2\text{O}$  equilibrium constant calculated by Hamilton and Naleway (1976).
8. Reaction 34 is required in the model to account for the excess radical initiation associated with all of our smog chamber experiments (Carter et al., 1979; Hendry et al., 1978). In modeling our  $\text{NO}_x$ -propene and/or n-butane-air chamber runs (Carter et al., 1979), we found that the values of  $k_{34}$  required for calculations to fit the data generally depended on initial  $\text{NO}$ ,  $\text{NO}_2$ , and humidity values. Based on these correlations (Carter et al., 1979; Carter, 1977-1978) the following values of  $k_{34}$  have been assigned:  $k_{34} \approx 0.2 \text{ ppb min}^{-1}$  for run 273;  $0.3 \text{ ppb min}^{-1}$  for runs 271 and 281; and  $0.4 \text{ ppb min}^{-1}$  for runs 266, 269, 293, 339, and 340.

9. The total  $\text{RO}_2 + \text{NO}$  rate constant used was assumed to be equal to that for the  $\text{CH}_3\text{O}_2 + \text{NO}$  rate constant  $k_{93}$ . Recently, Plumb et al. (1979) obtained a value of  $k_{93} = (8 \pm 2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ sec}^{-1}$  at room temperature, Adachi and Basco (1979) obtained  $k_{93} = (3.0 \pm 0.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ sec}^{-1}$  and Cox and Tyndall (1979) obtained  $(6.5 \pm 2.0) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ sec}^{-1}$ . Since Adachi and Basco (1979) may have had problems with the product  $\text{CH}_3\text{ONO}$  in their u.v. absorption system, and since  $\text{HO}_2$  formed from  $\text{HCO} + \text{O}_2$  may have caused problems in the study of Plumb et al. (1979), the data to date are ambiguous. We have used a value of  $k_{93}$  of  $8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ sec}^{-1}$ , identical to that for the reaction of  $\text{HO}_2$  radicals with  $\text{NO}$ , and consistent with the above-mentioned rate constant studies. The relative rates of alkoxy formation vs. alkyl nitrate formation are unknown for these systems, but based on the results of Darnall et al. (1976), alkyl nitrate formation probably occurs at least 10% of the time in  $\text{C}_5+$  systems. For these calculations the efficiency of alkyl nitrate formation was assumed to be the same for all  $\text{C}_6$  and  $\text{C}_7$  peroxy radicals, and the best fits to the data are obtained when ~25% alkyl nitrate formation is assumed. These reactions have also been discussed by Hoshino et al. (1978).
10. Ortho addition is assumed to predominate, based on experimental product data (Kenley et al., 1978; Hoshino et al., 1978; Grosjean et al., 1978), and results of the analogous addition of  $\text{O}(^3\text{P})$  atoms to toluene (Jones and Cvetanovic, 1961; Grovenstein and Mosher, 1970; Gaffney et al., 1976).
11. Reaction 42 is assumed to have the same rate constant as  $\text{RCH}_2\text{O} + \text{O}_2 \rightarrow \text{RCHO} + \text{HO}_2$  (e.g., reaction 96) since they have similar exothermicities (Benson, 1976) and probably have similar transition states.
12. Derived from  $k_{42}$  and the  $k_{42}/k_{43}$  ratio of Kenley et al., (1978). However, the nitrotoluene yields would be better fit if  $k_{43}/(k_{42} + k_{43} + k_{44} + k_{45})$  is a factor of ~10 higher.
13. The total rate constant of  $\text{O}_2$  addition to the toluene-OH adduct was the same for all mechanisms considered, and was adjusted to fit the observed maximum cresol yields in the runs modeled. Since the OH-aromatic- $\text{O}_2$  adduct can back-decompose to the  $\text{O}_2 +$  the OH-aromatic

adduct (Atkinson et al., 1979) or cyclize, this rate constant is a composite of  $k(O_2 + OH\text{-aromatic-adduct}) \times k(\text{cyclization})/k(\text{back-decomposition})$ . Since  $k(O_2 + OH\text{-aromatic-adduct})$  is expected, by analogy with other alkyl radicals, to be  $\sim 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ sec}^{-1}$  (Hampson and Garvin, 1978), this implies that the ratio of dissociation/cyclization for the OH-aromatic-O<sub>2</sub> adduct is  $\sim 300$ . This means that the OH-aromatic adduct and the OH-aromatic-O<sub>2</sub> adduct are probably essentially in equilibrium under atmospheric conditions.

14. Detailed reactions shown in Appendix B for substituent 2 = CH<sub>3</sub>, 1,3-6 = H.
15. The overall reaction occurs as shown if [2.2.2] cyclization predominates and re-cyclization is negligible (reactions 1'-6' in Appendix B).  $k_3'/(k_3' + k_4')$  is assumed to be 0.75.
16. Detailed reactions shown in Appendix B for substituent 6 = CH<sub>3</sub>, 1-4 = H.
17. The reaction occurs as shown if [3.2.1] cyclization predominates and re-cyclization is negligible (reactions 7'-15', 6' in Appendix B).  $k_9'/(k_9' + k_{10}')$  =  $k_{11}'/(k_{11}' + k_{12}')$  is assumed to be 0.75.
18. The reaction occurs as shown if re-cyclization predominates and if  $\beta$ -scission of  $\alpha$ -carbonyl,  $\beta$ -hydroxy alkoxy radicals results primarily in formation of carbonyl radicals. The same products are formed regardless of whether [3.2.1] or [2.2.2] cyclization predominates (reactions 1', 2', 7', 8', 16'-32').  $k_{21}'/(k_{21}' + k_{22}')$  =  $k_{23}'/(k_{23}' + k_{24}')$  is assumed to be 0.75.
19. The reaction occurs as shown if re-cyclization predominates and if  $\beta$ -scission of  $\alpha$ -carbonyl,  $\beta$ -hydroxy alkoxy radicals results primarily in formation of  $\alpha$ -hydroxy radicals. The same products are formed regardless of whether [3.2.1] or [2.2.2] cyclization predominates (reactions 1', 2', 7', 8', 16'-30', 33', 34', 6', 14').  $k_{21}'/(k_{21}' + k_{22}')$  =  $k_{23}'/(k_{23}' + k_{24}')$  is assumed to be 0.75.
20. Estimated from the observed disappearance rates of benzaldehyde in runs 337 and 339, after correcting for reaction of benzaldehyde with OH (Atkinson et al., 1979; Niki et al., 1978) and for benzaldehyde formation from OH + toluene (Atkinson et al., 1979; Perry et al., 1977a; Kenley et al., 1978). The hydroxyl radical concentrations were estimated using the toluene disappearance rates, and the OH + toluene rate constant (Atkinson et al., 1979; Perry et al., 1977a).

It is necessary to assume formation of nonradical products, or the overall reactivities of runs 337 and 339 are overpredicted.

21.  $\text{RCO}_3$  is assumed to react with NO with the same rate constant as  $\text{CH}_3\text{O}_2$  (see note 9). The  $k(\text{RCO}_3 + \text{NO})/k(\text{RCO}_3 + \text{NO}_2)$  ratio assigned by Carter et al. (1979) was used.
22. Assumed to occur with the same rate constant as that assigned for  $\text{RO}_2 + \text{HO}_2$  and  $\text{NO}_3 + \text{HO}_2$  (Carter et al., 1979).
23. OH addition as shown is estimated (Benson, 1976) to be at least 3-7 kcal mole<sup>-1</sup> more thermochemically favorable than addition at any other position, and is therefore assumed to predominate. Additionally, OH radical addition at this position yields the hydroxy nitrotoluene isomers observed for the different cresol isomers.
24. Assumed to have same rate constant as assigned for reaction 43 (see note 12).
25. Assumed to be analogous to  $\text{O}_3$  addition to the OH-toluene adduct, i.e.,  $k_{68} = k_{44}$  and  $k_{69} = k_{45}$  (see note 13).
26. Detailed reaction shown in Appendix B for substituent 1 = OH, 2 =  $\text{CH}_3$ , 3, 4, and 6 = H.
27. Detailed reactions shown in Appendix B for substituent 1 = OH, 6 =  $\text{CH}_3$ , 2-5 = H.
28. Included in the mechanism to account for the observed rapid disappearance of cresols in the presence of  $\text{O}_3 + \text{NO}_2$  (O'Brien, 1979; Carter et al., 1980), and the loss of cresol formed in  $\text{NO}_x$ -toluene-air runs following NO consumption. The rate constant was derived from subsidiary experiments (Carter et al., 1980). The mechanism is speculative, but its major feature is that net radical formation does not occur, since mechanisms which assume that  $\text{NO}_3 + \text{cresol}$  gives radicals result in significant overprediction of reactivity in  $\text{NO}_x$ -cresol-air runs.
29. Although glyoxal has large absorption coefficients in the 340-460 nm wavelength region (Calvert and Pitts, 1966) where the intensity of the photolyzing light is high, it appears to have low photodecomposition quantum yields at atmospheric pressure (Calvert and Pitts, 1966).
30. Assumed to react with a similar rate constant as other aldehydes (Atkinson et al., 1979).
31. This mechanism is assumed to be primarily H abstraction as shown

since OH radical addition to the double bond would be anticipated, by analogy with the reaction of O(<sup>3</sup>P) atom with acrolein and croton-aldehyde (Gaffney et al., 1975) [when compared to O(<sup>3</sup>P) and OH + ethene (Atkinson et al., 1979; Hampson and Garvin, 1978)] to have a rate constant of <5 x 10<sup>-12</sup> cm<sup>3</sup> molecule<sup>-1</sup> sec<sup>-1</sup>.

32. O<sub>3</sub> addition to the double bond is anticipated to be slow, by analogy with the reaction of O(<sup>3</sup>P) atoms with acrolein and crotonaldehyde (Gaffney et al., 1975) when compared to ethene (Atkinson et al., 1979; Hampson and Garvin, 1978).
33. The photochemistry of these species assumed to be analogous to that of acrolein and crotonaldehyde (Calvert and Pitts, 1966) which are believed to be photochemically stable under atmospheric conditions.
34. These initial additions to the double bond are estimated to be exothermic by ~3 kcal mole<sup>-1</sup>. If the estimates of Demerjian et al. (1974) (assuming an A factor of 10<sup>11.5</sup> sec<sup>-1</sup> and an activation energy of 11 kcal mole<sup>-1</sup>) are correct, these reactions should dominate over competing processes. However, if their activation energy estimate is low by ≥5 kcal mole<sup>-1</sup>, which is within the uncertainty range of their estimation, the reaction would be expected to be unimportant.
35. Nitrate formation is arbitrarily assumed to occur ~10% of the time, based on results for C<sub>4</sub> and C<sub>5</sub> alkyl radicals (Darnall et al., 1976).
36. Assumed to decompose with the same rate constant as peroxyacetyl-nitrate (PAN) (Hendry and Kenley, 1977; Cox and Roffey, 1977).
37. Assumed to occur with the same rate constant as OH + isopropanol (Atkinson et al., 1979).
38. Reaction with O<sub>2</sub> forming HO<sub>2</sub> and carbonyls has been shown to be the primary fate of α-hydroxy radicals in air [Carter et al., J. Phys. Chem. 83, 2305 (1979)].
39. The rates of photolysis for these acids are unknown. However, if it is assumed that they photolyze to form radicals rapidly (analogously to methylglyoxal), model calculations greatly overpredict the reactivity of the o-cresol-NO<sub>x</sub> system, regardless of which mechanistic option is used.
40. Assumed to react with the same rate constant as OH + toluene. This reaction is only significant in affecting primary nitrotoluene yields.

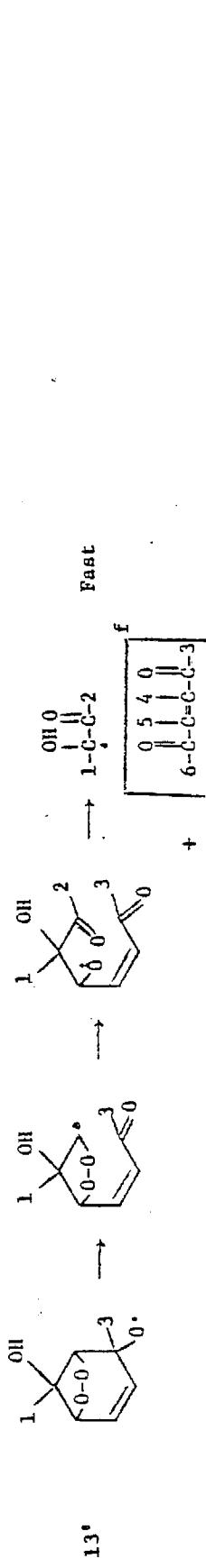
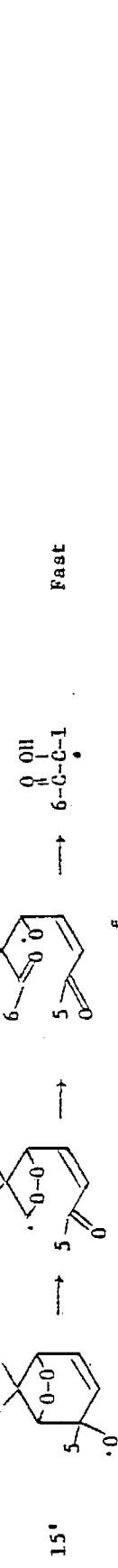
Appendix B. Reactions and Rate Constants for the General Aromatic-OH-O<sub>2</sub> Adduct System

Reaction	Rate constant cm <sup>3</sup> molecule sec units <sup>a,b</sup>	Mech. A-D, (G,H) <sup>d</sup> (Slow)	Mech. E,F	Notes <sup>c</sup>
<u>[2.2.2] Cyclization</u>				
			Fast	
<u>[2.2.2] Cyclization, No Re-cyclization</u>				
<u>[2.2.2] Cyclization, No Re-cyclization</u>				
<u>[2.2.2] Cyclization, No Re-cyclization</u>				
<u>[2.2.2] Cyclization, No Re-cyclization</u>				
<u>[2.2.2] Cyclization, No Re-cyclization</u>				
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<u>[2.2.2] Cyclization, No Re-cyclization</u>				
<u>[2.2.2] Cyclization, No Re-cyclization</u>				
<u>[2.2.2] Cyclization, No Re-cyclization</u>				
<u>[2.2.2] Cyclization, No Re-cyclization</u>				
<img alt="Chemical reaction scheme for cyclization of 4'. 4' is a benzene ring with substituents at positions 1, 2, 3, 4, 5, and 6. At position 1, there is a hydroxyl group (-OH) and a hydrogen atom. At position 2, there is a hydroperoxy radical (-OO·). At position 3, there is a hydrogen atom. At position 4, there is a double bond. At position 5, there is a hydrogen atom. At position 6, there is a hydrogen atom. An arrow points to a bicyclic adduct where the ring has closed at the				

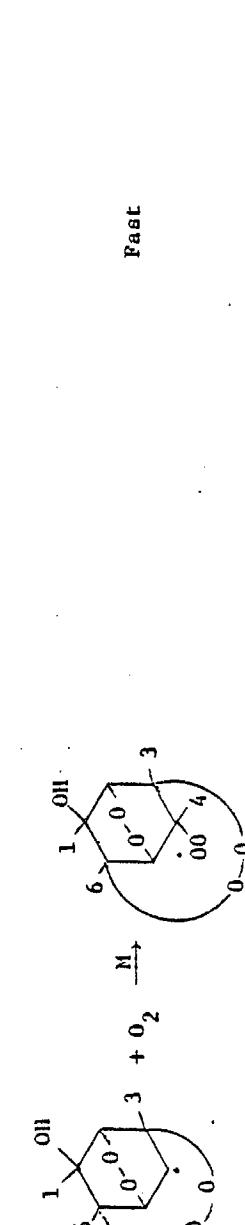
Appendix B. (cont.)

Reaction	Rate constant cm molecule sec units <sup>a,b</sup>	Mech. A-D	Mech. E,F,(G,H) <sup>d</sup>	Notes <sup>c</sup>
$6' \quad \begin{array}{c} \text{O} \\ \parallel \\ \text{OH} \\   \\ \text{6-C-1} \end{array} + \text{O}_2 \longrightarrow \boxed{\text{NO}_2 + \text{6-C-O-1}}$	Fast			38
<u>[3.2.1] Cyclization</u>				
$7' \quad \begin{array}{c} \text{OH} \\   \\ \text{6} \end{array} \begin{array}{c} \text{O} \\ \parallel \\ \text{OO} \cdot \\   \\ \text{2} \end{array} \begin{array}{c} \text{OH} \\   \\ \text{3} \end{array} \longrightarrow \begin{array}{c} \text{OH} \\   \\ \text{1} \end{array} \begin{array}{c} \text{O} \\ \parallel \\ \text{OO} \cdot \\   \\ \text{2} \end{array}$		(Slow)	Fast	
$8' \quad \begin{array}{c} \text{OH} \\   \\ \text{1} \end{array} \begin{array}{c} \text{O} \\ \parallel \\ \text{OO} \cdot \\   \\ \text{2} \end{array} \longrightarrow \begin{array}{c} \text{OH} \\   \\ \text{1} \end{array} \begin{array}{c} \text{O} \\ \parallel \\ \text{OO} \cdot \\   \\ \text{3} \end{array} + 1/2 \begin{array}{c} \text{OH} \\   \\ \text{1} \end{array} \begin{array}{c} \text{O} \\ \parallel \\ \text{OO} \cdot \\   \\ \text{5} \end{array}$	Fast			
<u>[3.2.1] Cyclization, No Re-cyclization</u>				
$9' \quad \begin{array}{c} \text{OH} \\   \\ \text{1} \end{array} \begin{array}{c} \text{O} \\ \parallel \\ \text{OO} \cdot \\   \\ \text{3} \end{array} + \text{NO} \longrightarrow \begin{array}{c} \text{OH} \\   \\ \text{1} \end{array} \begin{array}{c} \text{O} \\ \parallel \\ \text{OO} \cdot \\   \\ \text{3} \end{array} + \text{NO}_2$	$6 \times 10^{-12}$			
$10' \quad \begin{array}{c} \text{OH} \\   \\ \text{1} \end{array} \begin{array}{c} \text{O} \\ \parallel \\ \text{OO} \cdot \\   \\ \text{3} \end{array} + \text{NO} \xrightarrow{\text{M}} \begin{array}{c} \text{OH} \\   \\ \text{1} \end{array} \begin{array}{c} \text{O} \\ \parallel \\ \text{OO} \cdot \\   \\ \text{3} \end{array} \text{ONO}_2$	$2 \times 10^{-12}$	Ratio adjusted		9

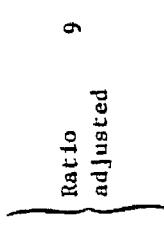
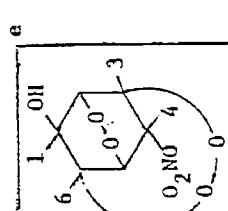
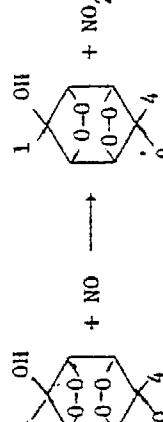
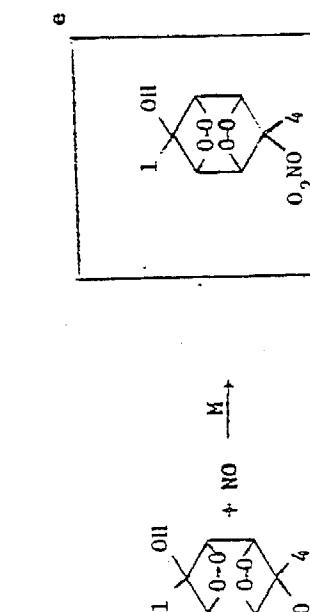
Appendix B. (cont.)

Reaction	Rate Constant cm molecule sec units <sup>a,b</sup>	Notes <sup>c</sup>
11'		6 x 10 <sup>-12</sup> Ratio adjusted 9
12'		2 x 10 <sup>-12</sup>
13'		Fast
14'		Fast
15'		Fast
		(Reaction 6')

Appendix B. (cont.)

	Reaction	Rate constant cm molecule sec <sup>c</sup> units <sup>a,b</sup>	Notes <sup>c</sup>
16*		$\left\{ \begin{array}{l} (\text{Slow}) \\ \text{Fast} \end{array} \right. \begin{array}{l} \text{Mech. A-F} \\ \text{Mech. G,H} \end{array}$	
17*		$\left\{ \begin{array}{l} (\text{Slow}) \\ \text{Fast} \end{array} \right. \begin{array}{l} \text{Mech. A-F} \\ \text{Mech. G,H} \end{array}$	
18*		$\left\{ \begin{array}{l} (\text{Slow}) \\ \text{Fast} \end{array} \right. \begin{array}{l} \text{Mech. A-F} \\ \text{Mech. G,H} \end{array}$	
19*			Fast
20*			Fast

Appendix B. (cont.)

Reaction	Rate constant cm molecule sec units <sup>a,b</sup>	Notes <sup>c</sup>
21'		$6 \times 10^{-12}$ 9
22'		$2 \times 10^{-12}$ 9
23'		$6 \times 10^{12}$ 9
24'		$2 \times 10^{12}$ 9

Appendix B. (cont.)

Reaction	Rate Constant cm molecule sec units <sup>a,b</sup>	Notes <sup>c</sup>
		$k_{25'} = k_{26'}$ Fast

Appendix B. (cont.)

Reaction	Rate constant cm molecule sec units <sup>a,b</sup>	Notes <sup>c</sup>
27'		Fast
28'		Fast
29'		Fast
30'		Fast
<u><math>\alpha</math>-Dicarbonyl Decomposition f</u>		
31'		<div style="display:flex; justify-content:space-around;"> <span>Fast</span> <span>Mech. G</span> </div> <div style="display:flex; justify-content:space-around;"> <span>(Slow)</span> <span>Mech. II</span> </div>
32'		<div style="display:flex; justify-content:space-around;"> <span>Fast</span> <span>Mech. G</span> </div> <div style="display:flex; justify-content:space-around;"> <span>(Slow)</span> <span>Mech. II</span> </div>

Appendix B. (cont.)

Reaction	Rate constant cm <sup>3</sup> molecule sec units <sup>a,b</sup>	Note <sup>c</sup>
<u><math>\beta</math>-Hydroxy Decomposition</u>		
33 <sup>d</sup>	$\begin{array}{ccc} \text{O} & \text{O} & \text{HO} \\   &   &    \\ \text{5}-\text{C}-\text{C}-\text{C}-2 & \longrightarrow & \boxed{\begin{array}{c} \text{O} \quad \text{O} \\    \quad    \\ \text{5}-\text{C}-\text{C}-6 \\   \\ 6 \quad 1 \end{array}} + \text{1-C-2} \end{array}$	$\left\{ \begin{array}{l} \text{(Slow)} \\ \text{Mech. G} \end{array} \right\}$ $\left\{ \begin{array}{l} \text{Fast} \\ \text{Mech. II} \end{array} \right\}$
34 <sup>e</sup>	$\begin{array}{ccc} \text{O} & \text{OH} & \text{O} \\   &   &    \\ \text{6}-\text{C}-\text{C}-\text{C}-3 & \longrightarrow & \boxed{\begin{array}{c} \text{O} \quad \text{O} \\    \quad    \\ \text{6}-\text{C}-\text{C}-1 \\   \\ 1 \quad 2 \end{array}} + \boxed{\begin{array}{c} \text{O} \quad \text{O} \\    \quad    \\ \text{2}-\text{C}-\text{3} \end{array}} \end{array}$	$\left\{ \begin{array}{l} \text{(Slow)} \\ \text{Mech. G} \end{array} \right\}$ $\left\{ \begin{array}{l} \text{Fast} \\ \text{Mech. II} \end{array} \right\}$
	$\begin{array}{ccc} \text{HO} & \text{O} & \text{f} \\   &   &    \\ \text{1-C-2} & + \text{O}_2 & \longrightarrow \boxed{\begin{array}{c} \text{O} \quad \text{O} \\    \quad    \\ \text{HO}_2 + \text{1-C-2} \end{array}} \end{array}$	Fast (Reaction 14 <sup>f</sup> )
	$\begin{array}{ccc} \text{O} & \text{OH} & \text{f} \\   &   &    \\ \text{6}-\text{C}-\text{C}-1 & + \text{O}_2 & \longrightarrow \boxed{\begin{array}{c} \text{O} \quad \text{O} \\    \quad    \\ \text{HO}_2 + \text{6}-\text{C}-\text{1} \end{array}} \end{array}$	Fast (Reaction 6 <sup>f</sup> )

<sup>a</sup> Rate constants are given for the conditions of the smog chamber runs listed in Appendix A ( $T = 303$  K, 735 torr, M = air). Photolysis rate constants are given for the light intensity and spectral distributions associated with runs 327-340 (Pitts et al., 1979b); photolyses rate for runs 266-281 are somewhat lower.

<sup>b</sup> First order reaction:  $\text{sec}^{-1}$ ; 2nd order reaction:  $\text{cm}^3 \text{molecule}^{-1} \text{sec}^{-1}$ ; "fast" means that the reaction is the sole pathway for that particular species; the predictions are insensitive for the actual rate constant. "(Slow)" means that the reaction is assumed to be negligible, or that the reaction has a negligible effect on the predictions of the model for the concentration regimes studied here.

<sup>c</sup> Footnotes are those of Appendix A.

<sup>d</sup> Mechanisms G and II predict formation of same products regardless of whether [2.2.2] or [3.2.2] cyclization occurs.

<sup>e</sup> Subsequent reactions of this product are ignored.

<sup>f</sup> Subsequent reactions of these species or intermediates are shown in Appendix A.

## V. INVESTIGATION OF THE EFFECT OF TEMPERATURE ON PHOTOCHEMICAL SMOG FORMATION

The formation of photochemical smog is influenced by a number of meteorological factors whose natural fluctuations contribute to the observed variations in frequency and intensity of episodes at different locations and times of year. Among the most important factors from a fundamental gas phase chemical kinetic standpoint is temperature. Although there has recently been considerable progress in understanding the temperature dependencies of the many individual elementary processes occurring in photochemical smog mechanisms, there has been very limited data available for the purpose of testing the temperature-dependent aspects of these kinetic mechanisms in their entirety. Analysis of air quality data is not particularly useful in this regard because conditions of lower temperature are usually also associated with conditions of reduced light intensity or duration, both of which are known to significantly affect photochemical smog formation. Smog chamber studies are potentially more useful for elucidating temperature effects, but the amount of smog chamber data obtained at varying temperatures has been highly limited, and the impact of chamber effects on temperature dependencies observed in such experiments has not been adequately characterized.

In order to satisfy the need for well characterized smog chamber data suitable for the validation of models of the effect of temperature on photochemical smog formation, a series of variable temperature chamber experiments has been performed employing the SAPRC evacuable chamber-solar simulator facility. This included the irradiation of surrogate hydrocarbon- $\text{NO}_x$ -air mixtures at average temperatures of 8°C, 30°C and 51°C, and, for control purposes, alkane- $\text{NO}_x$ -air mixtures at the same temperatures. The alkane system is chosen as a control because its chemistry is reasonably well understood (Carter et al., 1979). Efforts have been made to assure that these experiments are well characterized, with experimental variables unrelated to temperature effects, such as light intensity and characteristics, reactant injections, moisture content, etc. held constant. A description of the experimental design and procedures, and the results of the 14 surrogate and the 10 control irradiations are given below.

Experimental Design. The composition of the surrogate hydrocarbon mixture employed in this study is given in Table 14. It is based on the mixture previously employed in SAPRC-ARB chamber experiments (Pitts et al., 1975; 1976a; 1979a) which was designed to represent the ambient air pollutant burden from all sources in the South Coast Air Basin. The hydrocarbon mixture was modified to include n-hexane as a representative of the longer chain alkanes, which are missing in the previous surrogate mixture. (Recent results have shown that because of the possibility of a rapid, 1,5-H shift isomerization of sufficiently long alkoxy radicals, the reactions of the longer alkanes in photochemical smog conditions are not analogous to those of, for example, n-butane or 2,3-dimethylbutane.) The relative concentrations of n-hexane and the other alkanes in the modified surrogate were chosen so that (1) the total ppmC of alkane relative to the other types of hydrocarbons was the same as in the previous SAPRC-ARB surrogate mixture, and (2) the ratios of the different types of labile C-H bonds was the same as those for the alkanes listed by Calvert for an 8:30 a.m. LARPP Los Angeles sample (Calvert, 1976). (Primary, secondary, tertiary, and C-H bonds that can, after reacting with OH, O<sub>2</sub> and NO, form alkoxy radicals which undergo the rapid 1,5-H shift isomerization, were counted as separate types.) An additional modification of the hydrocarbon mixture was that the oxygenates were represented entirely by acetaldehyde rather than primarily by formaldehyde; this was done to simplify and make more reproducible the hydrocarbon reactant injections.

Another modification of the reactant mixtures relative to the previous surrogate programs was that in the initial NO<sub>x</sub> mixture, NO<sub>2</sub> was increased from 10% to 25%. This makes the NO<sub>2</sub>:NO ratio more consistent with early morning monitoring data, and is what is assumed in the EPA EKMA model (Dodge, 1977b).

The composition of the control alkane-NO<sub>x</sub> runs consisted of equal amounts of n-butane and neopentane as the reactant hydrocarbons, with the initial NO<sub>x</sub> approximately 25% NO<sub>2</sub>. n-Butane was chosen because its mechanism has been reasonably well validated (Hendry et al., 1978; Carter et al., 1979), with its major uncertainties being attributed to chamber effects. A dual rather than a single alkane system is preferred because

Table 14. Composition of Surrogate Hydrocarbon Mixture  
Used in Temperature Effects Study

Hydrocarbon	Mole %	% Carbon
<u>Alkanes</u> -- Total	<u>64.0</u>	<u>65.3</u>
Ethane	13.0	6.5
Propane	5.8	4.4
n-Butane	27.6	27.8
2,3-Dimethylbutane	9.3	14.1
n-Hexane	8.3	12.5
<u>Olefins</u> -- Total	<u>13.3</u>	<u>10.1</u>
Ethene	6.8	3.4
Propene	1.9	1.4
cis-2-Butene	2.4	2.4
2-Methyl-2-butene	2.2	2.8
<u>Aromatics</u> -- Total	<u>9.2</u>	<u>17.9</u>
Toluene	2.7	4.8
m-Xylene	6.5	13.1
<u>Alkynes</u>		
Acetylene	<u>8.2</u>	<u>4.1</u>
<u>Oxygenates</u>		
Acetaldehyde	<u>5.2</u>	<u>2.6</u>

the change in the ratios of the two alkanes with time gives a good technique to estimate hydroxyl radical concentrations without the necessity to correct for dilution. Neopentane was chosen as the second alkane because it is the least reactive alkane which can reliably be analyzed on the same chromatographic column as n-butane, allowing changes in their ratio to be determined with maximum precision. Neopentane reactions account for less than 24% of the hydrocarbon consumed, and its mechanism is expected to be analogous to that of n-butane and other alkanes; therefore its presence should introduce no major uncertainties.

The blocks of surrogate- $\text{NO}_x$ -air and control n-butane/neopentane- $\text{NO}_x$ -air runs were done at varying hydrocarbon and  $\text{NO}_x$  levels, with each experiment performed at both high ( $51^\circ\text{C}$ ) and low ( $8^\circ\text{C}$ ) temperatures. In addition, representative surrogate and n-butane/neopentane runs were done at  $30^\circ\text{C}$ . The experimental protocol was such that surrogate and n-butane/neopentane runs, and runs with different initial hydrocarbon and  $\text{NO}_x$  levels were dispersed so that chamber memory effects, if any, should not have a systematic impact on the data.

Experimental Procedures. All experiments in this program were performed in the SAPRC 6800-liter, thermostatted evacuable smog chamber. The evacuable chamber, the solar simulator light source, and the pure air system employed have been described previously (Beauchene et al., 1973; Doyle et al., 1977; Winer et al., 1980). In these experiments, continuous monitoring was done using a Dasibi  $\text{O}_3$  analyzer, and using simultaneously a TECO 14B and a newly acquired TECO 14B/E chemiluminescent  $\text{NO-NO}_x$  analyzer. Chromatographic samples were taken at 15-45 minute intervals for analysis of reactant hydrocarbons, PAN and oxygenated products; samples for analysis of formaldehyde using the chromotropic acid technique were taken hourly. The intensity of the photolyzing light was monitored by periodic  $\text{NO}_2$  actinometry experiments, and its relative spectral distribution was determined for each experiment by a spectrometer-photomultiplier system. The experimental and analytical procedures and techniques used in these experiments were those generally employed in our evacuable chamber programs reported elsewhere (Pitts et al., 1979a,b), except as noted below.

For all runs temperature control was maintained to within  $\pm 1^\circ\text{C}$  and

$k_1$  for  $\text{NO}_2$  photolysis was held constant at  $0.39 \text{ min}^{-1}$ . The spectral distribution of the photolyzing light did not change significantly throughout the program. Regardless of the temperature of the run, purified air was humidified to ~15% RH at ambient temperature ( $\sim 30^\circ\text{C}$ ) prior to entering the chamber; this corresponds to ~5% RH at  $51^\circ\text{C}$  and ~60% RH at  $8^\circ\text{C}$ .

Efforts were made to minimize the introduction of nitrous acid (HONO) into the chamber during injection of  $\text{NO}_x$  by removing moisture HONO and other impurities from the NO and  $\text{NO}_2$  used, and by not allowing high concentrations of NO or  $\text{NO}_2$  to be exposed to each other or to water vapor prior to and during the injection procedure. Because of the potential of initially present HONO, due to its rapid photolysis, to affect the results of the irradiation, the  $\text{NO}_x$  purification and injection procedures are described in detail and were used for all runs in this study.

NO was purified by passing it through a trap containing Linde Molecular Sieve 13X cooled to  $-98^\circ\text{C}$  with a methanol slush. The contents of the trap were previously dried by being flushed with dry  $\text{N}_2$  at  $300^\circ\text{C}$ .  $\text{NO}_2$  was prepared by reaction of ~100 torr of the purified NO with ~1 atm of excess  $\text{O}_2$  overnight, followed by trapping the  $\text{NO}_2$  formed by pumping the reaction mixture through a liquid  $\text{N}_2$ -cooled trap. The  $\text{O}_2$  used to make the  $\text{NO}_2$  was previously dried by being passed through a Linde Molecular Sieve 13X-filled trap cooled with liquid Ar. Both the purified NO and the synthesized  $\text{NO}_2$  were stored in bulbs (darkened for  $\text{NO}_2$ ) attached to a conventional high vacuum rack interfaced directly to the evacuable chamber.

NO and  $\text{NO}_2$  were introduced into the evacuated chamber prior to the fill of the chamber with humidified air, as follows. On the day prior to the experiment, the desired pressures of NO and  $\text{NO}_2$  were placed in separate ~5 liter bulbs of accurately known volumes attached both to the chamber and the vacuum rack. The chamber was evacuated to  $< 10^{-5}$  torr and pumped overnight. On the day of the run, the chamber was filled to  $\sim 10^{-20}$  torr with dry  $\text{N}_2$ , followed by flushing the NO into the chamber with  $\text{N}_2$ . After the NO was completely injected, the  $\text{NO}_2$  was injected through a separate port into the chamber.

Similar high vacuum techniques were also used in introducing surrogate hydrocarbon mixture into the chamber in order to obtain greater reproducibility in hydrocarbon injection. All hydrocarbon reactants in the surrogate

mixture except the liquids 2-methyl-2-butene and m-xylene were pre-mixed and stored in the gas phase in a Pyrex bulb. Appropriate pressures in accurately known volumes of this "gas surrogate" mixture and the m-xylene and 2-methyl-2-butene were mixed the day before the experiment and stored in a liquid N<sub>2</sub> cooled trap prior to being flushed into the chamber with N<sub>2</sub>. Surrogate injection was done after NO<sub>x</sub> injection but prior to the pure air fill. For the alkane runs, neopentane and n-butane were injected using syringes after the pure air fill.

Results. The initial reactant concentrations, temperature, and humidity for the experiments are summarized in Table 15 for the surrogate runs and in Table 16 for the alkane control runs. Table 17 summarizes the levels of reproducibility, average values and standard deviations of initial reactant concentrations, temperatures, and humidity in runs where duplicate values were desired.

The 6-hr ozone values and the estimated average hydroxyl (OH) radical concentrations obtained in these runs are shown in Tables 18 and 19. Both the 6-hr ozone value and the estimated average OH levels increase significantly with increasing temperature. For both the surrogate and the control runs, the average OH levels increase by factors of 3 to 4 with increase in temperature from 8°C to 50°C. The OH levels observed for 30°C are approximately the geometrical mean of the corresponding runs ~22°C warmer or cooler.

Detailed tabulations of the reactant and product data, and of the physical parameters monitored during these runs are given in Appendix D. In order to facilitate the utilization of these data in model validations, they will be made available on magnetic tape in computer readable format upon request. A description of the organization of the tape and associated computer usage will be provided with the tape.

Discussion. Since the primary purpose of this study is to provide data suitable for model validation, a full discussion of the implications of the results presented here of the effects of temperature on photochemical smog formation must await the results of model calculations simulating these runs. However, several observations can be made without the benefit of such calculations.

Table 15. Initial Reactant Concentration, Average Temperature, Humidity and Water Content of Surrogate Hydrocarbon- $\text{NO}_x$ -Air Evacuable Chamber Runs

Run No.	Avg. Temp. (°C)	$\text{H}_2\text{O}^a$ ( $10^3$ ppm)	Humid- ity <sup>b</sup> (%)	Initial Concentrations				
				$\text{NO}^c$ (ppm)	$\text{NO}_2^c$ (ppm)	$\text{NO}_x^c$ (ppm)	NMHC <sup>d</sup> (ppmC)	CO (ppm)
362	29.6	4.3	20	0.082	0.029	0.111	0.67	0.6
365	7.9	6.7	63	0.072	0.027	0.099	0.68	2.4
366	51.7	5.2	5	0.078	0.034	0.111	0.71	0.4
367	49.3	6.3	5	0.097	0.021	0.118	0.46	0.4
368	8.7	1.7	29	0.068	0.033	0.102	0.44 <sup>e</sup>	0.3
371	8.9	5.2	34	0.033	0.025	0.058	2.00 <sup>e</sup>	1.4
372	51.6	6.1	5	0.040	0.023	0.063	1.96	0.2
375	8.2	5.0	38	0.210	0.079	0.289	1.94	- <sup>f</sup>
376	51.1	6.6	5	0.248	0.091	0.339	2.37	0.7
379	7.9	5.2	49	0.067	0.027	0.094	2.17	-
380	52.3	6.2	5	0.076	0.034	0.110	2.40	-
381	51.5	5.2	5	0.035	0.020	0.055	0.50	-
382	7.8	3.3	32	0.029	0.020	0.046	0.43	-
387	28.9	6.1	17	0.073	0.034	0.107	0.79	0.7

<sup>a</sup>Calculated from the wet and dry bulb temperature at the time of the pure air fill.

<sup>b</sup>Calculated from the average temperature and the initial  $\text{H}_2\text{O}$  temperature using  $\text{H}_2\text{O}$  vapor pressures.

<sup>c</sup>Average of readings from TECO 14B/1 and 14B/E chemiluminescent  $\text{NO}-\text{NO}_x$  monitors.

<sup>d</sup>Calculations based on the measured initial concentrations of the injected ethane, propane, n-butane, 2,3-dimethylbutane, n-hexane, ethene, propene, cis-2-butene, 2-methyl-2-butene, toluene, m-xylene, acetylene, and acetaldehyde.

<sup>e</sup>Data values for acetaldehyde missing. NMHC calculated using intended initial acetaldehyde concentrations.

<sup>f</sup>- No data taken.

Table 16. Initial Reactant Concentration, Average Temperature, Humidity and Water Content of Alkane-NO<sub>x</sub>-Air Evacuable Chamber Runs

Run No.	Avg. Temp. (°C)	H <sub>2</sub> O <sup>a</sup> (10 <sup>3</sup> ppm)	Humid-ity <sup>b</sup> (%)	Initial Concentrations					
				NO <sup>c</sup> (ppm)	NO <sub>2</sub> <sup>c</sup> (ppm)	NO <sub>x</sub> <sup>c</sup> (ppm)	n-Butane (ppmC)	Neo-pentane (ppm)	CO (ppm)
360	7.5	5.7	51	0.368	0.123	0.495	2.75	2.81	-e
361	51.9	6.1	5	0.392	0.132	0.524	2.83	2.81	1.1
363	25.9	5.2	20	0.153	0.060	0.213	1.49	1.50	0.3
369	7.5	4.3	33	0.138	0.052	0.190	1.42	1.39	0.8
370	51.2	5.5	5	0.157	0.062	0.219	1.55	1.55	0.8
373	7.6	4.4	31	0.350	0.125	0.475	1.40	1.40	0.7
374	50.8	5.6	5	0.391	0.137	0.528	1.55	1.57	-
383	9.5	6.3	41	0.030	0.022	0.052	1.39	1.39	0.3
384	50.2	6.9	5	0.037	0.019	0.056	1.64	1.64	0.6
386	29.6	5.2	14	0.147	0.058	0.204	1.54	1.53	0.4

<sup>a</sup>Calculated from the wet and dry bulb temperature at the time of the pure air fill.

<sup>b</sup>Calculated from the average temperature and the initial H<sub>2</sub>O temperature using H<sub>2</sub>O vapor pressures.

<sup>c</sup>Average of readings from TECO 14B/1 and 14B/E chemiluminescent NO-NO<sub>x</sub> monitors.

<sup>d</sup>Calculations based on the measured initial concentrations of the injected ethane, propane, n-butane, 2,3-dimethylbutane, n-hexane, ethene, propene, cis-2-butene, 2-methyl-2-butene, toluene, m-xylene, acetylene, and acetaldehyde.

e- No data taken.

Table 17. Intended and Observed Average Values and Observed Standard Deviations of Initial Reactant and Water Concentrations and Temperature Measurements in Comparable Evacuable Chamber Runs

Quantity Measured	Desired Value	Observed Value	No. Runs	Desired Value	Observed Value	No. Runs	Desired Value	Observed Value	No. Runs
Temperature (°C)	8°C	8.2 ± 0.7	10	30°C	28.5 ± 1.8	4	51°C	51.2 ± 0.9	10
H <sub>2</sub> O(10 <sup>3</sup> ppm) <sup>a</sup>	~6	5.3 ± 1.2	24	—	—	—	—	—	—
RH (%)	-60	44 ± 13	10	-15	14 ± 4	4	-5	4.6 ± 0.6	10
<u>Initial Concentrations</u>									
NO (ppm) <sup>b</sup>	0.038	0.034 ± 0.006	6	0.075	0.077 ± 0.020	8	0.150	0.149 ± 0.012	4
NO <sub>2</sub> (ppm)	0.013	0.021 ± 0.004	6	0.025	0.030 ± 0.009	8	0.050	0.058 ± 0.004	4
NO <sub>x</sub> (ppm)	0.050	0.055 ± 0.009	6	0.100	0.107 ± 0.014	8	0.200	0.207 ± 0.017	4
NO (ppm)	0.225	0.23 ± 0.03	2	0.375	0.38 ± 0.02	4	—	—	—
NO <sub>2</sub> (ppm)	0.075	0.08 ± 0.01	2	0.125	0.129 ± 0.01	4	—	—	—
NO <sub>x</sub> (ppm)	0.300	0.31 ± 0.03	2	0.500	0.51 ± 0.02	4	—	—	—
n-Butane (ppm) <sup>c</sup>	1.5	1.59 ± 0.09	8	3.0	2.79 ± 0.05	2	—	—	—
Neopentane (ppm) <sup>c</sup>	1.5	1.49 ± 0.09	8	3.0	2.898 ± 0.002	2	—	—	—
Total Surrogate (ppmC) <sup>d</sup>	0.45	0.46 ± 0.03	4	0.70	0.73 ± 0.06	4	2.2	2.1 ± 0.2	6
<u>Surrogate Components (ppb)<sup>d</sup></u>									
Ethane	14.6	16.7 ± 1.0	4	22.8	25.8 ± 1.3	3	71.5	68 ± 10	6
Propane	6.6	8.4 ± 0.6	4	10.3	12.1 ± 0.6	4	32.3	36 ± 2	6
n-Butane	31.3	32.9 ± 2.7	4	48.7	50.6 ± 2.5	4	152.9	162 ± 11	6
2,3-Dimethylbutane	10.6	10.7 ± 0.8	4	16.5	16.9 ± 1.4	4	51.7	54 ± 4	6
n-Hexane	9.4	9.5 ± 0.5	4	14.6	14.4 ± 0.8	4	45.8	47 ± 4	6
Ethene	7.7	5.6 ± 1.1	4	11.9	12.9 ± 1.2	3	37.4	31 ± 6	6
Propene	2.1	2.3 ± 0.2	4	3.3	3.5 ± 0.2	4	10.3	11.3 ± 1.0	6
cis-2-Butene	2.7	2.5 ± 0.2	4	4.2	4.0 ± 0.3	4	13.2	13 ± 2	6
2-Methyl-2-butene <sup>e</sup>	2.5	2.3 ± 0.3	4	3.9	3.5 ± 0.3	4	12.3	11.6 ± 2	6
Toluene	3.1	3.1 ± 0.8	4	4.8	5.0 ± 1.1	4	15.1	14.3 ± 1.0	6
m-Xylene <sup>e</sup>	7.4	6.9 ± 0.4	4	11.5	10.8 ± 1.0	4	36.0	34 ± 8	5
Acetylene	9.2	11.5 ± 0.7	4	14.4	16.8 ± 0.5	3	45.1	47 ± 7	6
Acetaldehyde	5.9	4.9 ± 1.1	2	9.1	12.3 ± 3.1	3	28.6	18 ± 5	5

<sup>a</sup>Calculated from the wet and dry bulb temperature at the time of the pure air fill.

<sup>b</sup>Average of readings from TECO 14B/1 and TECO 14B/E chemiluminescent NO-NO<sub>x</sub> monitors.

<sup>c</sup>Alkane runs only.

<sup>d</sup>Surrogate runs only.

<sup>e</sup>Injected separately from other components of the mixture, so greater variability relative to the other components expected.

Table 18. Six-Hour Ozone and Estimated Hydroxyl Levels Observed in Surrogate- $\text{NO}_x$ -Air Evacuable Chamber Experiments

Nominal Initial Concentrations <sup>a</sup> NMHC $\text{NO}_x$ (ppmC)	$T = 8^\circ\text{C}$			$T = 30^\circ\text{C}$			$T = 51^\circ\text{C}$		
	Run No.	6-hr $O_3$ (ppm)	Est. $[\text{OH}]^b$ (molec $\text{cm}^{-3}$ )	Run No.	6-hr $O_3$ (ppm)	Est. $[\text{OH}]^b$ (molec $\text{cm}^{-3}$ )	Run No.	6-hr $O_3$ (ppm)	Est. $[\text{OH}]^b$ (molec $\text{cm}^{-3}$ )
0.45 0.05	382	0.068	$4.4 \times 10^6$				381	0.237	$1.3 \times 10^7$
0.45 0.1	368	0.039	$2.3 \times 10^6$				367	0.237	$9.5 \times 10^6$
0.7 0.1	365	0.056	$3.1 \times 10^6$	{ 362      0.176 $5.8 \times 10^6$ } { 387      0.167 $5.6 \times 10^6$ }			366	0.327	$1.2 \times 10^7$
2.2 0.05	371	0.085 <sup>c</sup>	$3.1 \times 10^6$				372	0.359	$6.0 \times 10^6$
2.2 0.1	379	0.176 <sup>c</sup>	$1.4 \times 10^6$				380	0.477	$7.8 \times 10^6$
2.2 0.3	375	0.044	$2.1 \times 10^6$				376	0.576	$7.6 \times 10^6$

<sup>a</sup>Concentrations given are desired initial concentrations. Actual initial concentrations may be slightly different.

<sup>b</sup>Calculated from the relative decay rates of n-butane and 2,3-dimethylbutane using  $k(\text{OH} + \text{n-butane}) = 2.8 \times 10^{-12}$   $\text{cm}^3 \text{ molecule}^{-1} \text{ sec}^{-1}$  and  $k(\text{OH} + 2,3\text{-DMB}) = 5.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ sec}^{-1}$ .

<sup>c</sup>Maximum  $O_3$  observed prior to 6 hours.

Table 19. Six-Hour Ozone and Estimated Hydroxyl Levels Observed in Alkane- $\text{NO}_x$ -Air Evacuable Chamber Experiments

Nominal Initial Concentrations <sup>a</sup>	$T = 8^\circ\text{C}$			$T = 30^\circ\text{C}$			$T = 51^\circ\text{C}$		
	Run No.	6-hr $\text{O}_3$ (ppm)	Est. $[\text{OH}]^c$ (molec $\text{cm}^{-3}$ )	Run No.	6-hr $\text{O}_3$ (ppm)	Est. $[\text{OH}]^c$ (molec $\text{cm}^{-3}$ )	Run No.	6-hr $\text{O}_3$ (ppm)	Est. $[\text{OH}]^c$ (molec $\text{cm}^{-3}$ )
Alkane <sup>b</sup> (ppm)									
$\text{NO}_x$ (ppm)									
3 0.05	383	0.098	$7 \times 10^5$				384	0.391	$1.8 \times 10^6$
3 0.2	369	0.042	$6 \times 10^5$	{ 363 386 }	>0.076 <sup>d</sup> 0.196	$1.1 \times 10^6$ $1.3 \times 10^6$	{ 370 374 }	0.696 0.332	$3.0 \times 10^6$ $2.0 \times 10^6$
3 0.5	373	0.010	$5 \times 10^5$						
6 0.5	360	0.027	$6 \times 10^5$				361	0.989	$2.3 \times 10^6$

<sup>a</sup>Concentrations given are initial concentrations desired. Actual initial concentrations may be slightly different.

<sup>b</sup>Given as concentration of neopentane + n-butane (ppm). Equal quantities of each used.

<sup>c</sup>Calculated from the relative decay rates of n-butane and neopentane using  $k(\text{OH} + \text{n-butane}) = 8.7 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ sec}^{-1}$ , and  $k(\text{OH} + \text{neopentane}) = 8.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ sec}^{-1}$ .

<sup>d</sup>4-hour value. Compare with 4-hour  $\text{O}_3$  value of 0.098 ppm for EC-386.

The data in Tables 18 and 19 indicate that temperature strongly affects radical levels in both the surrogate- $\text{NO}_x$  and the alkane- $\text{NO}_x$  runs. Much, if not all, of the effect of temperature on ozone formation can be attributed to this increase of radical levels with temperature, since it is the radical propagation reactions converting NO to  $\text{NO}_2$  which are responsible for  $\text{O}_3$  build-up. Therefore, an understanding of the cause of the strong effect of temperature on radical levels is important to understanding the effect of temperature on photochemical smog formation.

The increase in radical levels with temperature could be due to increasing rates of radical initiation reactions, or to decreasing rates of radical termination processes, or to a combination of both. Prior to the consumption of  $\text{NO}_x$ , the major termination reactions are radical +  $\text{NO}_2$  reactions forming nitrates or peroxy nitrates. In the alkane system the major known radical initiation processes are ozone and aldehyde photolysis (Demerjian et al., 1974; Hendry et al., 1978; Carter et al., 1979). In the surrogate system, reactions of ozone with olefins and photolysis of the  $\alpha$ -dicarbonyls will also contribute to initiation, and the higher radical levels observed in surrogate runs can be rationalized on the basis of these reactions. Although the radical levels in the surrogate runs are on the average over four times higher than those of alkane runs at the same temperature, the relative increase in OH concentration with temperature increase from  $8^\circ\text{C}$  to  $30^\circ\text{C}$  and from  $30^\circ\text{C}$  to  $51^\circ\text{C}$  is the same in both systems. This suggests that the cause of the strong effect of temperature on radical levels is in some aspect of the mechanism common to both systems.

In the alkane- $\text{NO}_x$  system, where the major organic photooxidation products can be monitored, it is possible to estimate the total extent of initiation or termination from the known processes. Estimates are made using (1) observed yields of termination products (e.g., alkyl nitrates and PAN), (2) estimations of average OH +  $\text{NO}_2$  rates using average measured  $\text{NO}_2$  values and estimated OH levels, and (3) integrated  $\text{O}_3$  and oxygenate yields and calculated photolysis rate constants for the photolysis conditions. Such estimates are given in Table 20 for three representative alkane- $\text{NO}_x$  runs with similar initial reactant concentrations at the three temperatures studied. At all three temperatures the total amount of

Table 20. Estimated Integrated Initiation and Termination Rates from Known Processes in Representative Alkane-NO<sub>x</sub>-Air Chamber Runs

Temperature (°C)	8	30	51	Notes
EC Run No.	369	386	370	
6-hr Integrated Rates (ppb radicals)				
<u>Initiation - Total</u>	<u>9</u>	<u>15</u>	<u>50</u>	
$O_3 + h\nu \xrightarrow{H_2O} 2 OH + O_2$	0.4	2	10	a,b
HCHO + hν → Radicals	4	5	19	b,c
CH <sub>3</sub> CHO + hν → Radicals	1	2	8	b,c
CH <sub>3</sub> CH <sub>2</sub> COCH <sub>3</sub> + hν → Radicals	3	3	5	b,c
CH <sub>3</sub> COCH <sub>3</sub> + hν → Radicals	1	3	8	b,c
<u>Termination - Total</u>	<u>17</u>	<u>56</u>	<u>241</u>	
OH + NO <sub>2</sub> $\xrightarrow{M}$ HNO <sub>3</sub>	11	36	205	d
CH <sub>3</sub> CO <sub>3</sub> + NO <sub>2</sub> $\xrightarrow{M}$ PAN	1	12	26	e
Radicals + NO <sub>x</sub> → RONO <sub>2</sub>	5	8	10	e
<u>Excess Initiation</u>				
6-hr Integrated Rate (ppb)	8	41	191	
Avg. Rate (ppb min <sup>-1</sup> )	0.02	0.1	0.5	

- a) Estimated from the measured 6-hr O<sub>3</sub> dose, the calculated rate of O<sub>3</sub> photolysis to O<sup>1</sup>D, and the O<sup>1</sup>D rate constants (Hampson & Garvin, 1978) as shown below:

$$\int_0^{360} (\text{rate OH input}) dt = 2 \left[ \int_0^{360} [O_3] dt \right] k (O_3 \xrightarrow{h\nu} O^1D) \frac{k(O^1D + H_2O)}{k(O^1D + H_2O + k(O^1D + M))}$$

- b) These estimates used photolysis rate constants for O<sub>3</sub> (to O<sup>1</sup>D) for formaldehyde, acetaldehyde, and ketone respectively of  $2 \times 10^{-3}$ ,  $9 \times 10^{-4}$ ,  $2 \times 10^{-4}$ , and  $4 \times 10^{-4}$  sec<sup>-1</sup>. These were calculated from the appropriate absorption coefficients, quantum yields, measured intensities, and spectral distribution of the photolyzing light in these runs. Absorption coefficients and quantum yields for O<sub>3</sub> and formaldehyde used are those recommended by

Table 20. (Continued)

Hampson & Garvin (1978) and Horowitz & Calvert (1978), respectively. Acetaldehyde and ketone absorption coefficients and quantum yields were those of Calvert & Pitts (1966); acetaldehyde quantum yields were those of Weaver et al. (1977); and ketone photolysis to radicals was assumed to be 100% efficient.

- c) Estimated from the measured integrated aldehyde yield and the appropriate photolysis rate constant as shown

$$\int_0^{360} (\text{rate, radical input}) dt = 2 \left[ \int_0^{360} [\text{RCHO}] dt \right] k(\text{RCHO} + h\nu \rightarrow \text{radical})$$

- d) Estimated from the measured average  $[\text{NO}_2]$ , the estimated average  $[\text{OH}]$  (Table 19) and the  $\text{OH} + \text{NO}_2$  rate constant (Hampson & Garvin, 1978) as shown

$$\int_0^{360} \text{rate } (\text{OH} + \text{NO}_2) dt \approx k (\text{OH} + \text{NO}_2) [\text{OH}]_{\text{avg}} \int_0^{360} [\text{NO}_2] dt$$

- e) Integrated rate identified with the observed yields of the appropriate product(s). "RONO<sub>2</sub>" includes primarily methyl and butyl nitrates.

termination is significantly greater than the total amount of initiation from known processes, with the discrepancy increasing strongly with temperature. Since initiation and termination must balance, there is an unknown radical source which becomes greater with increasing temperature.

The existence of unknown radical sources in smog chamber systems is now generally recognized (Bufalini et al., 1977; Falls and Seinfeld, 1978; Hendry et al., 1978; Whitten et al., 1979; Carter et al., 1979) and is a serious problem in modeling such systems. It is frequently attributed to photolysis of HONO formed during the injection of  $\text{NO}_x$  through the interaction of NO and  $\text{NO}_2$  with water vapor (Chan et al., 1976); but, as discussed above,  $\text{NO}_x$  injection in this study was done in such a way as to minimize HONO formation. In any case, it is unclear how HONO photolysis could be the cause of the observed increase of the unknown radical source with temperature. In order for the concentration of HONO to be sufficient to affect the system, it must be fairly close to equilibrium with NO,  $\text{NO}_2$  and  $\text{H}_2\text{O}$ , but the equilibrium HONO actually decreases with temperature (Benson, 1976). Thus, the nature of the temperature-dependent radical source is unknown, though it appears likely that it is due to offgassing of some highly photoreactive contaminant from the chamber walls. It is reasonable to expect such offgassing to increase with increasing temperature.

Additional evidence for the increased importance of contaminant offgassing at higher temperatures comes from the fact that in the 51°C runs, the total  $\text{NO}_x$  consumption is considerably less than what would be expected on the basis of estimated rates of the  $\text{OH} + \text{NO}_2$  reaction. Decreased  $\text{NO}_x$  consumption could be attributed in part to increased  $\text{HNO}_3$  interferences on the chemiluminescent  $\text{NO}_x$  monitor (Winer et al., 1974) due to less efficient adsorption of  $\text{HNO}_3$  vapor on the walls of the sampling tubes at higher temperature, but in a number of 51°C runs the total monitored  $\text{NO}_x$  actually increased. Because of the uncertainties in the  $\text{NO}_x$  measurements introduced by the possibility of a semi-quantitative  $\text{HNO}_3$  interference, the exact magnitude of the offgassing cannot be determined from these data. It is quite possible that the unknown radical source and the evidence for  $\text{NO}_x$  offgassing at high temperatures are related, since offgassing of a highly photoreactive nitrogen-containing species such as

HONO or alkyl nitrites could account for both effects.

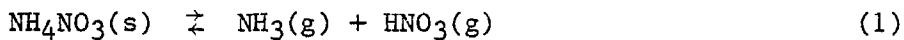
Conclusions and Future Research. There is a major effect of temperature on photochemical smog simulations in smog chamber systems, but current evidence suggests that most of this could be an artifact introduced by chamber effects. Until chamber effects relating to radical initiation are more completely understood, it will not be possible to unambiguously validate photochemical models concerning temperature effects using smog chamber data. More chamber characterization experiments are required, particularly those with more quantitative data concerning offgassing at higher temperatures.

We are conducting studies in the ongoing SAPRC-ARB chamber program on the effect of temperature on photochemical smog formation in which relative humidity will be varied. Because the data reported here suggest that chamber effects may play a dominant role in these experiments, additional chamber characterization and control experiments will be incorporated into the program. Contaminant offgassing will be studied as a function of temperature and humidity both in the dark and during irradiation. It is hoped that these additional experiments will increase the level of characterization, and thus the utility, of the experiments reported here.

## VI. STUDIES OF THE RELATIONSHIPS BETWEEN AMBIENT AMMONIA AND NITRIC ACID AND PARTICULATE NITRATE: IMPLICATIONS FOR NITRATE ARTIFACT FORMATION

The need to reliably establish ambient levels of ammonium nitrate particulates in ambient air (National Academy of Sciences, 1978) and the evidence for "artifact effects" (Witz and MacPhee, 1977; Spicer and Schumacher, 1977; Spicer, 1977; Spicer and Schumacher, 1978; Appel et al., 1979; Meserole, 1978) in widely used sampling methods for particulate nitrate have led to recent interest in the roles that the precursors ammonia and nitric acid play in the formation of ammonium nitrate in the atmosphere and on filters. Unfortunately, direct and simultaneous measurements of ammonia and nitric acid in ambient air have previously been unavailable. Indeed, the only data of a related nature are the pairs of 1-hr maxima for  $\text{NH}_3$  and  $\text{HNO}_3$  concentrations in West Covina reported by Spicer (1974), who employed microcoulometric and modified chromotropic acid (colorimetric) techniques for  $\text{HNO}_3$  and dual-catalyst chemiluminescence detection for  $\text{NH}_3$ .

Stelson, Friedlander, and Seinfeld (1979) recently utilized these data (Spicer, 1974) in an analysis of the applicability of the equilibrium relationship in Equation 1 to the atmosphere. We wish to extend this



analysis using simultaneous, absolute concentrations of  $\text{NH}_3$  and  $\text{HNO}_3$  in ambient air, which we measured with short (<6 min) integration times in Riverside, California, in 1977 using a kilometer path-length Fourier transform infrared (FT-IR) spectrometer (Tuazon et al., 1978; Tuazon et al., 1980).

Experimental. High-resolution FT-IR spectra of ambient air have been obtained during air pollution episodes in the California South Coast Air Basin at a downwind site (Riverside) during 1976 and 1977 (Pitts et al., 1979a) using a long-path FT-IR system and experimental methods that have been previously described (Tuazon et al., 1978; Tuazon et al., 1980). The system consists of a Digilab Model 196 interferometer ( $0.5 \text{ cm}^{-1}$  maximum resolution) interfaced to an eight-mirror long-path cell with a 22.5-m base path and capable of achieving kilometer path lengths. The cell optics are

gold-coated for maximum reflectivity in the infrared, and a HgCdTe liquid- $N_2$  cooled detector was employed for the 700-2000  $\text{cm}^{-1}$  region. The detection limits for  $\text{NH}_3$  and  $\text{HNO}_3$  afforded by this facility for a 5-min scanning interval are 4 and 6 ppb, respectively, and the average uncertainty in each quantity is approximately one-half of the detection limit. From 249 spectra, 54 instances were found where the concentrations of both ammonia and nitric acid were above the detection limits. These cases were found among spectra taken at half-hour intervals between late morning and early evening during air pollution episodes in the months of July to October, 1977. Temperature and relative humidity data were obtained from instruments operating in the ACHEX laboratory (Appel et al., 1978) immediately adjacent to the kilometer path-length FT-IR facility. During selected episodes, 24-hr high-volume particulate samples were also collected on washed Gelman AE glass fiber filters and were subsequently analyzed for ammonium, nitrate, and sulfate ions by the indophenol blue (Weatherburn, 1967), cadmium reduction-diazotization, and turbidimetric methods, respectively.

Results. The data employed in the present analysis are given in Table 21 and plotted in Figure 44. These data met two conditions: (1) concentrations of both  $\text{NH}_3$  and  $\text{HNO}_3$  exceeded the detection limits, and (2) measurements were made during high oxidant episodes (i.e.,  $\text{O}_3 \geq 100$  ppb). Relative humidity never exceeded 50% during these observations and did not correlate significantly with concentration data. Temperatures given in Table 21 are interpolated to the times of the spectral observations from readings recorded at 10-min intervals.

The mass concentrations determined for the  $\text{NH}_4^+$ ,  $\text{NO}_3^-$ , and  $\text{SO}_4^{=}$  ions from particulate data are given in Table 22. Multiple linear regressions using these data and a much larger data block obtained at the same sampling site during the previous two years (Pitts and Grosjean, 1978) suggest that the mixture consists of ammonium nitrate and two sulfates of ammonia. A recent field study of high-volume sampling artifacts for particulate inorganics (Mischke, 1979) indicates small positive errors for nitrate ( $\lesssim 15\%$ ) and a probable negative error for ammonium for 24-hr samples obtained from highly polluted air at Riverside on Gelman AE filters.

Table 21. Ambient Concentrations of Ammonia and Nitric Acid from Kilometer Path-Length FT-IR Spectroscopic Measurements

1977 (Date)	Time (PST)	NH <sub>3</sub> (ppb)	HNO <sub>3</sub> (ppb)	Temp. (°C)
7/21	1434	24	10	36.2
	1452	19	7	35.5
	1510	13	9	35.0
	1532	11	10	34.2
	1611	6	10	33.0
	1718	9	12	32.4
7/25	1523	18	20	37.6
	1542	19	17	37.3
	1604	13	15	36.4
	1622	14	12	36.3
	1655	13	14	35.5
8/11	1057	13	8	31.3
	1400	37	8	36.0
	1435	21	13	35.4
	1454	14	10	34.6
	1516	16	10	34.2
	1535	13	9	34.2
	1553	10	11	33.5
	1616	9	9	32.9
8/12	1132	15	16	33.2
	1202	33	11	34.0
	1230	38	9	34.4
	1300	46	9	35.0
	1400	29	9	35.8
	1430	32	9	35.5
	1459	22	9	34.5
	1529	20	10	34.0
	1603	13	11	33.0
	1612	9	10	32.2
	1640	4	8	31.5
9/9	1113	17	9	33.5
	1132	13	8	33.1
	1200	16	8	34.7
	1235	47	6	35.3
10/3	1300	25	10	33.6
	1405	54	9	33.7
10/4	1500	37	8	33.5
	1530	28	9	31.9

Table 21. (continued)

1977 (Date)	Time (PST)	NH <sub>3</sub> (ppb)	HNO <sub>3</sub> (ppb)	Temp. (°C)
10/11	1224	6	12	30.1
	1244	5	9	30.9
	1333	59	8	32.9
10/14	1230	23	9	35.2
	1330	102	7	35.7
	1400	93	8	34.7
	1424	55	8	33.8
	1444	46	8	33.7
10/17	1202	15	9	29.6
	1231	20	11	29.6
	1300	27	9	30.5
10/18	1411	16	6	27.3
10/26	1130	5	10	27.3
	1202	6	8	28.2
	1231	9	8	31.3
	1300	24	8	30.5

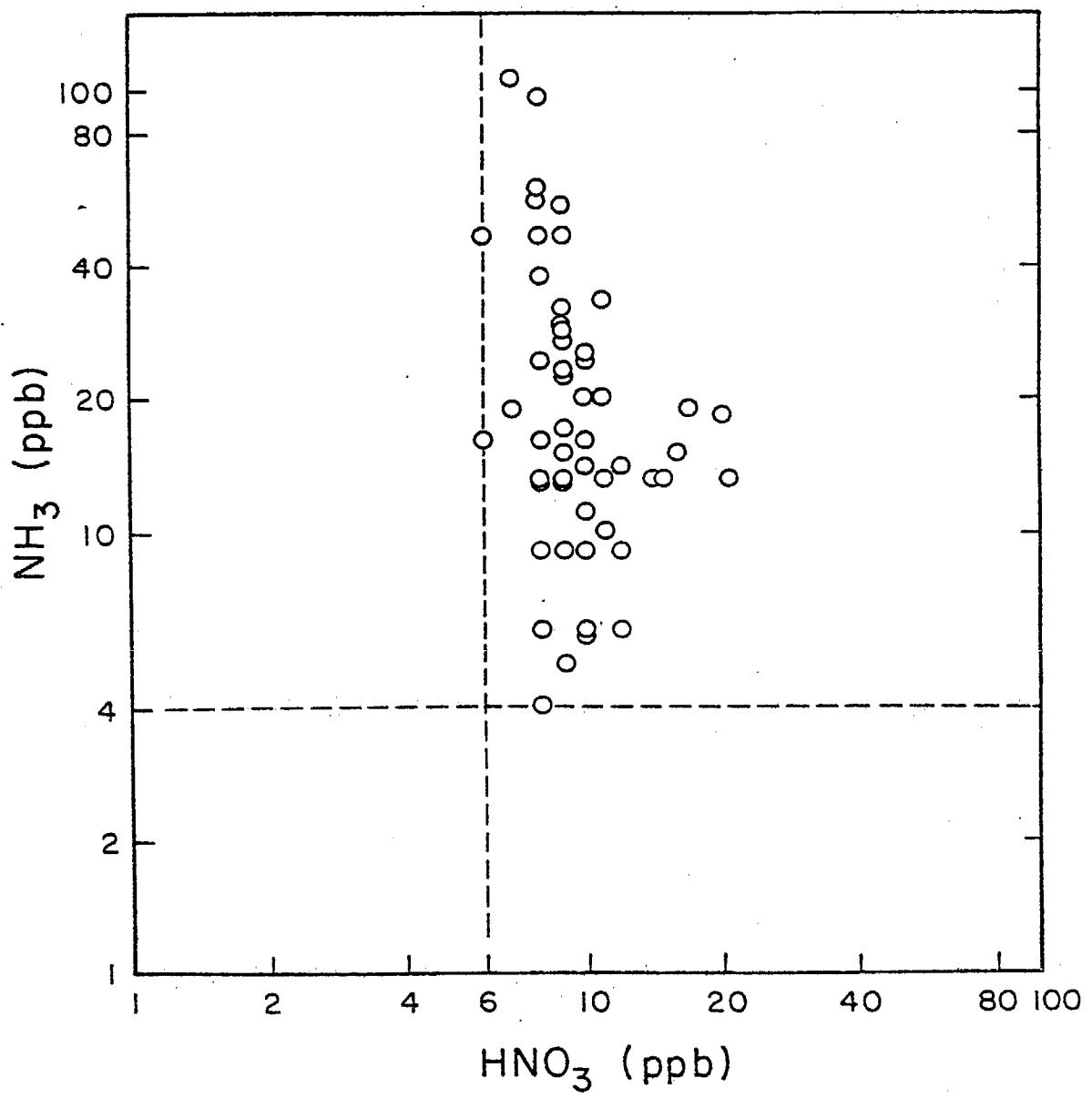


Figure 44. Distribution of Simultaneous Observations of Ammonia and Nitric Acid Concentrations: (---) Detection Threshold.

Table 22. Particulate Analyses of 24-hr Samples

Date (1977)	Mass Concentration ug m <sup>-3</sup>			
	NH <sub>4</sub> <sup>+</sup>	NO <sub>3</sub> <sup>-</sup>	SO <sub>4</sub> <sup>=</sup>	NH <sub>4</sub> NO <sub>3</sub> <sup>a</sup>
7/21	13	42	12	54
7/25	4	18	13	29
8/11	17	60	25	77
8/12	14	50	20	64
9/09	2	21	NI <sup>b</sup>	27
10/03	18	67	18	86
10/04	NI	NI	NI	NI
10/11	20	65	6	84
10/14	16	50	21	64
10/17	27	74	26	96
10/18	33	86	31	111
10/26	20	64	16	83

<sup>a</sup>Ammonium nitrate equivalent to nitrate ion data.<sup>b</sup>NI means no information available.

Consequently, the best estimates of ammonium nitrate concentrations can be calculated from the nitrate data and are given in the fifth column of Table 22. A more extensive analysis of data for particulate samples at this site is given by Pitts and Grosjean (1978). Although the data in Table 22 are averages for 24-hr periods, the presence of particulate ammonium nitrate seems probable during many, if not all, periods when FT-IR spectra were obtained.

A small negative correlation (-0.31 with a 95% confidence level for the range -0.53 to -0.05) between the NH<sub>3</sub> and HNO<sub>3</sub> concentrations in Table 21 indicates qualitatively that these concentrations are being affected by chemical reaction or an equilibrium relationship (i.e., Equation 1), since the concentrations of two noninteracting pollutants are usually positively correlated as a result of common meteorological influences. Strict adherence to the equilibrium of Equation 1 would give a hyperbolic

relationship between the  $\text{NH}_3$  and  $\text{HNO}_3$  concentrations and a correlation coefficient between -1.0 and 0.0. In this case the values of the coefficient depends on the variance of the independent variable, and approaches zero for very large variances. The logarithm of the  $\text{NH}_3\text{-HNO}_3$  concentration product has a significant positive correlation with temperature (e.g., +0.55 with a 95% confidence level for the range +0.33 to 0.71), as expected for the  $\text{NH}_4\text{NO}_3$  equilibrium. The data are insufficient, however, to resolve any dependence of the logarithm of the concentration production on humidity.

The effect of temperature on the logarithmic concentration products at these low to moderate humidities is well represented by a regression coefficient of about  $0.2 \text{ deg}^{-1}$ . This is consistent with the concentration product representing an equilibrium constant for solid particulate, which is the probable state of ammonium nitrate containing particles at these temperatures and humidities (i.e., RH < 55%) (Dingemans, 1941). The temperature dependence of the equilibrium relationship of Equation 1 from thermochemical data is compared to our experimental data in the scatter diagram shown in Figure 45. The means of the concentration product and temperature data and their least-squares regression coefficients are given in Table 23 as changes in the free energy and enthalpy for Reaction 1; the same quantities, as estimated from compilations of thermochemical data, are also given in Table 23 for comparison.

It should be noted that temperatures were not measured directly in the FT-IR multiple reflection cell but were inferred from adjacent ambient air measurements. Deviation of up to  $1^\circ\text{C}$  were possible, which can have significant effects when the enthalpy change is  $\sim 44 \text{ kcal}$ .

Discussion. Much of the difference between the enthalpy change calculated from the regression slope of our experimental data and the enthalpy change from thermochemical data (see Table 23) may be due to deviations from ambient temperature in the outdoor FT-IR cell. Since temperature deviations are affected by diurnal variations of such factors as radiation intensity and wind speed, they may not be completely random and can result in a bias. The regression coefficient estimate is quite sensitive to bias in the independent variable (in this case temperature), and thus the enthalpy change calculated from our data could contain a systematic error.

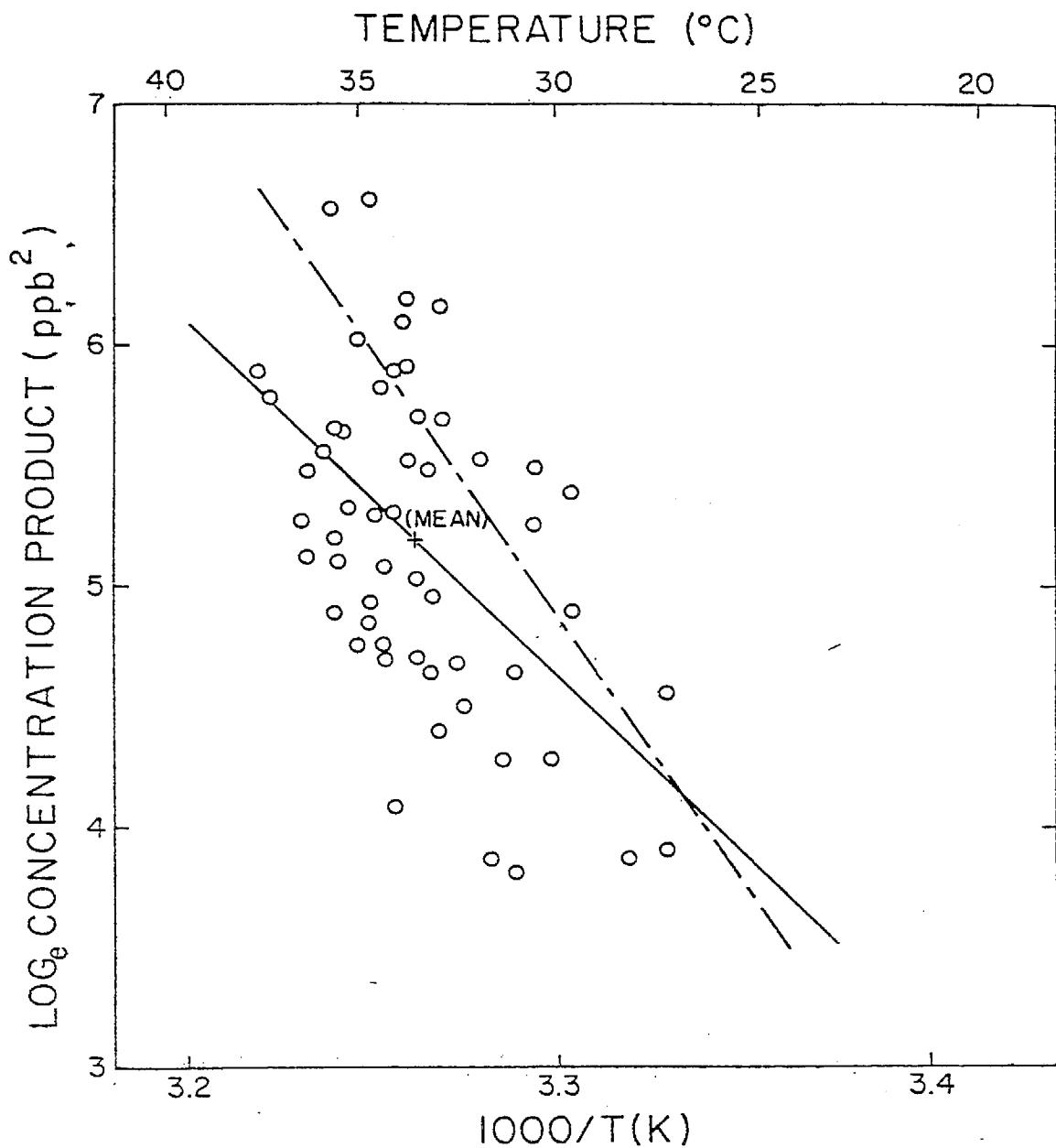


Figure 45. Logarithm of the  $\text{NH}_3\text{-HNO}_3$  Concentration Product vs. the Reciprocal Absolute Ambient Temperature: (—) Regression Line Calculated from Unweighted Experimental Data (54 Observations); (---) Regression Line Calculated from Thermodynamic Data.

Table 23. Thermodynamic Data for the  $\text{NH}_4\text{NO}_3$  Equilibrium at 306.6 K<sup>a</sup>

	Derived from Experimental Data <sup>b</sup>	Calculated from Thermodynamic Data <sup>c</sup>
Free-energy Change, kcal/mol	22.08 ( $\pm 0.12$ )	21.78
Enthalpy Change, kcal/mol	30 ( $\pm 12$ )	43.79

<sup>a</sup>Average of all temperatures in these experiments.

<sup>b</sup>The temperature and free-energy change are the means of the 54 observations. Enthalpy is calculated from the slope of the unweighted regression line. The uncertainties in parentheses are 95% confidence intervals.

<sup>c</sup>Calculated at 306.6 K from heat of formation data given by JANAF Tables (Stull and Prophet, 1971) and by Wagman et al. (1968) using gas heat capacities from Benson (1968) and solid heat capacities from Wagman et al. (1968). The small heat of transition contribution for  $\text{NH}_4\text{NO}_3$  at 305.4 K was included ( $\Delta H = 0.410$  kcal/mol).

The free-energy change is calculated from the mean of all our observations, and this quantity is thus both much more precise than the enthalpy change and less sensitive to systematic temperature errors. The very good agreement (see Table 23) between the free-energy change calculated from our  $\text{NH}_3$  and  $\text{HNO}_3$  data and that from tabulated thermodynamic data may be somewhat fortuitous; the presence of possible bias due to several factors such as lack of ammonium nitrate saturation for some air samples or errors in temperature measurements cannot be ruled out. Surface effects would tend to lower the experimental free-energy change, but the characteristic particle size of nitrate in the eastern end of the South Coast Air Basin is fairly large (e.g., ~0.5 m) and particle destabilization due to the free energy of the surface should be negligible (i.e., <0.02 kcal/mol). Moreover, most ammonium nitrate containing particles in a polluted atmosphere are probably impure, and the adsorption of impurities and water vapor tends to reduce thermodynamic surface effects.

Stelson et al. (1979) compared the  $\text{NH}_4\text{NO}_3$  equilibrium constant calculated from thermodynamic data to some gas-phase  $\text{HNO}_3$  and  $\text{NH}_3$  data collected at West Covina by Spicer (1974). Although no equilibrium constant was calculated from the experimental data, a plot showed reasonable agreement with the equilibrium constant from thermodynamic data (Stelson et al., 1979)

and with  $\text{NH}_4\text{NO}_3$  dissociation pressure measurements by Brandner et al. (1962). Since experimental data presented here were obtained at a mean temperature of 306.6 K, a small heat of transition for a  $\text{NH}_4\text{NO}_3$  phase change at 305.4 K was included in the calculations using thermodynamic data (see Table 23). The experimental data and thermodynamics calculations presented here are in good agreement with the conclusions of Stelson et al. (1979) and support the hypothesis that gaseous ammonia and nitric acid are in equilibrium with solid ammonium nitrate in the atmosphere.

The probable existence of this equilibrium in a polluted atmosphere has direct utility for the calculation of particulate nitrate concentrations from chemical models. However, its implications for nitrate-sampling artifacts are unclear. Transfer of ammonium nitrate to and from a filter sample via the precursors involves a fairly complex mass transfer process at the interface; the rate of this process seems quite sensitive to surface conditions. In a few experiments it was found that impure nitrate in atmospheric filter samples volatilized into a simulated sampling flow of precursor-free air much more slowly than pure ammonium nitrate on a filter (Meserole, 1978; Mischke, 1979). Inhibition of volatilization implies inhibition of condensation, and thus further investigation into nitrate sampling artifacts is needed.

Conclusion. Although subject to uncertainties in temperature and in particulate composition for individual air samples, our observations support the hypothesis that particulate ammonium nitrate is in equilibrium with its precursors, ammonia and nitric acid. Atmospheric measurements under more carefully controlled conditions and a precise, direct determination of the thermodynamic data for Reaction 1 would be required for complete confirmation. Nonetheless, the ammonium nitrate equilibrium constant derived from tabulated thermochemical data is consistent with our atmospheric measurements of  $\text{NH}_3$  and  $\text{HNO}_3$  and is of direct utility in atmospheric models for calculating particle nitrate concentrations.

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APPENDIX C

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BAG-101  
DUAL OUTDOOR BAG DMAE SURFGATE RUN #1  
1979 APR 4

TIME (PDT)  
0600-0820 BAG # 11 (WITH NO DIVIDING BARI) FILLED WITH CHAMBER PURÉ AIR.

0800 BAG COVERED

0930-1015 61107 200 MICROLITERS (U-L) DMAE INJECTED  
13.1 ppm in bag, calculated  
1310 1.6 ml no injected  
1312 4 ml no2 injected  
1516 BAG UNCOVERED  
1723-1746 HI VOL (FREE FLOW) USED TO EMPTY CONTENTS (APP 40 CUBIC METERS)  
1130 RH IS 34% AT 32.5 DEG C (OUTDOOR TEMPERATURE)

GC-MS SAMPLES TAKEN:

1004-1014 #1 (5.0 L)  
1453-1504 #2 6 #3 (BACKUP) (5.9 L)  
1540-1600 #4 6 #4 (BACKUP) (4.6 L)  
1711-1741 #5 6 #5 (BACKUP) (5.5 L)  
DAS 181 1790 AND BENODIX USED

\*MEASUREMENTS SO MARKED INCLUDE THE FOLLOWING UNITS AND FACTORS:

B-SCAT (METERS-1) X E+4  
CONDENSATION NUCLEI (PART/CUBIC CM) X E-3  
AEROSOL NUMBER (PART/CUBIC CM) X E-3  
AEROSOL SURFACE (U-METERS2/CUBIC CM) X E-2  
AEROSOL VOLUME (CUBIC U-METERS/CUBIC CM) X 1  
UV (CAL/CM2-MIN) X 1

T=0 AT 1200 PDT

TS DEG K AVERAGE  
UV AVERAGE 300.0  
0.004

\* ASSIGNED INITIAL CONDITION

BAG-101  
DUAL DUTYOR BAG CHME SURROGATE RUN #1  
1979 APR 4

CLOCK TIME	ELAPSED TIME (MIN)	OZONE ppm	OZONE ppm	NC ppm	NO2-CORR ppm	NOX-CORR ppm
042	-198.	0.018	0.003	0.0	0.002	0.007
055	-185.	***	***	***	*****	*****
020	-160.	***	***	***	*****	*****
049	-131.	0.037	0.003	0.0	0.003	0.0
055	-125.	***	***	***	*****	*****
1035	-85.	0.011	0.001	0.0	0.0	0.003
1055	-75.	***	***	***	*****	*****
1124	-36.	0.028	0.001	0.0	0.0	0.0
1130	-30.	***	***	***	*****	*****
1155	-5.	***	***	***	*****	*****
1215	15.	***	***	***	*****	*****
1230	30.	***	***	***	*****	*****
1255	55.	***	***	***	*****	*****
1325	85.	0.005	0.002	0.322	0.078	0.384
1350	110.	***	***	***	*****	*****
1400	120.	0.004	0.005	0.278	0.076	0.340
1415	135.	***	***	***	*****	*****
1430	150.	0.011	0.004	0.249	0.078	0.318
1500	180.	0.015	0.001	***	*****	*****
1530	210.	0.020	0.003	0.246	0.036	0.321
1600	240.	***	***	***	*****	*****
1605	245.	0.047	0.004	0.249	0.111	0.345
1630	270.	0.047	0.004	0.247	0.111	0.345
1645	285.	***	***	***	*****	*****
1700	300.	0.041	0.005	0.257	0.120	0.357
1734	334.	0.040	0.002	0.315	0.120	0.413

BAG-101  
DUAL OUTDOOR BAG DMAE SURROGATE RUN #1  
1979 APR 4

CLOCK TIME	ELAPSED TIME (MIN)	DMAE PPM	ACETALD PPM	PROPALD PPM	ACETONE PPM	MEK PPM	METHANE PPM	ETHANE PPM	ETHENEF PPM	ACETYLEN PPM	PROPANE PPM	PROPENE PPM	I-C4 PPM
842	-198.	*****	*****	*****	*****	0.0005	*****	*****	0.0047	*****	*****	*****	*****
355	-185.	0.001	0.001	0.0003	0.0003	0.0013	1.42	0.0017	0.0094	0.0014	0.0018	0.001	0.0004
920	-160.	0.0005	0.0005	0.0005	0.0005	0.0005	*****	*****	*****	*****	*****	*****	*****
949	-131.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
955	-125.	0.0009	0.0009	0.0009	0.0009	0.0009	*****	*****	*****	*****	*****	*****	*****
1035	-85.	0.0014	0.0014	0.0014	0.0014	0.0014	*****	*****	*****	*****	*****	*****	*****
1055	-65.	0.0013	0.0013	0.0013	0.0013	0.0013	*****	*****	*****	*****	*****	*****	*****
1124	-36.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1130	-30.	0.2898	0.2898	0.2898	0.2898	0.2898	*****	*****	*****	*****	*****	*****	*****
1155	-5.	0.6444	0.6444	0.6444	0.6444	0.6444	*****	*****	*****	*****	*****	*****	*****
1215	1.5.	0.7495	0.7495	0.7495	0.7495	0.7495	*****	*****	*****	*****	*****	*****	*****
1230	3.0.	0.7615	0.7615	0.7615	0.7615	0.7615	*****	*****	*****	*****	*****	*****	*****
1255	5.5.	0.7987	0.7987	0.7987	0.7987	0.7987	*****	*****	*****	*****	*****	*****	*****
1325	85.	0.8049	0.8049	0.8049	0.8049	0.8049	*****	*****	*****	*****	*****	*****	*****
1350	11.0.	0.7801	0.7801	0.7801	0.7801	0.7801	*****	*****	*****	*****	*****	*****	*****
1400	120.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1415	135.	0.7975	0.7975	0.7975	0.7975	0.7975	*****	*****	*****	*****	*****	*****	*****
1430	150.	0.7721	0.7721	0.7721	0.7721	0.7721	*****	*****	*****	*****	*****	*****	*****
1500	180.	*****	*****	0.005	0.005	0.0011	1.41	0.0003	0.0184	0.0011	0.0110	0.0015	0.0002
1530	210.	0.7938	0.7938	0.7938	0.7938	0.7938	*****	*****	*****	*****	*****	*****	*****
1600	240.	0.6847	0.6847	0.6847	0.6847	0.6847	*****	*****	*****	*****	*****	*****	*****
1605	245.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1630	270.	0.7636	0.7636	0.7636	0.7636	0.7636	*****	*****	*****	*****	*****	*****	*****
1645	285.	*****	*****	0.007	0.007	0.0003	0.0015	0.0005	0.0057	0.0058	0.0021	0.0036	0.0009
1700	300.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1734	334.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****

BAG-101  
DUAL OBJECTOR BAG DMAE SURROGATE RUN #1  
1979 APR 4

CLOCK TIME	ELAPSED TIME (MIN)	N-C <sub>4</sub> PPM	1-C <sub>4</sub> = PPM	1-C <sub>5</sub> PPM	BENZENE PPM	TOLUENE PPM
8'42	-19d.	*****	*****	*****	*****	*****
855	-185.	0.001	0.0002	0.0013	0.0004	0.001
920	-160.	*****	*****	*****	*****	*****
949	-131.	*****	*****	*****	*****	*****
955	-125.	*****	*****	*****	*****	*****
1035	-85.	*****	*****	*****	*****	*****
1055	-65.	*****	*****	*****	*****	*****
1124	-36.	*****	*****	*****	*****	*****
1130	-30.	*****	*****	*****	*****	*****
1155	-5.	*****	*****	*****	*****	*****
1215	1.5.	*****	*****	*****	*****	*****
1230	3.0.	*****	*****	*****	*****	*****
1255	55.	*****	*****	*****	*****	*****
1325	35.	*****	*****	*****	*****	*****
1350	11.0.	*****	*****	*****	*****	*****
1400	12.0.	*****	*****	*****	*****	*****
1415	13.5.	*****	*****	*****	*****	*****
1430	15.0.	*****	*****	*****	*****	*****
1500	100.	0.000	0.0002	0.0003	0.0002	0.000
1530	21.0.	*****	*****	*****	*****	*****
1600	24.0.	*****	*****	*****	*****	*****
1605	24.5.	*****	*****	*****	*****	*****
1630	27.0.	*****	*****	*****	*****	*****
1645	28.5.	0.002	0.0	0.0013	0.0004	0.001
1700	30.0.	*****	*****	*****	*****	*****
1734	33.4.	*****	*****	*****	*****	*****

BAG-101  
DUAL OUTDOOR BAG DMAE SURROGATE RUN #1  
1979 APR 4

CLOCK TIME	ELAPSED TIME	B-SCAT	CONDENS.	AEROSL N	AEROSL S	AEROSL V	TS	DEG F	UV
842	-198.	* 0.40	* 0.0	* 2.47	* 0.54	* 2.10	71.5	*****	*****
855	-185.	*****	*****	*****	*****	*****	*****	****	****
920	-160.	*****	*****	*****	*****	*****	****	****	****
949	-131.	0.30	3.00	9.01	0.99	1.73	77.1	*****	*****
955	-125.	*****	*****	*****	*****	*****	****	****	****
1035	-85.	0.30	3.90	9.37	2.38	5.79	81.4	*****	*****
1055	-65.	*****	*****	*****	*****	*****	****	****	****
1124	-36.	0.30	3.40	9.03	2.85	8.03	81.9	*****	*****
1130	-30.	*****	*****	*****	*****	*****	****	****	****
1155	-5.	*****	*****	*****	*****	*****	****	****	****
1215	1.5.	*****	*****	*****	*****	*****	****	****	****
1230	3.0.	*****	*****	*****	*****	*****	****	****	****
1255	5.5.	*****	*****	*****	*****	*****	****	****	****
1325	85.	0.70	11.00	24.10	0.78	27.10	83.9	*****	*****
1350	11.0.	*****	*****	*****	*****	*****	****	****	****
1400	12.0.	0.55	8.50	22.10	7.93	26.00	83.6	*****	*****
1415	13.5.	*****	*****	*****	*****	*****	****	****	****
1430	15.0.	0.80	8.00	19.50	8.26	28.60	84.3	*****	*****
1500	180.	0.85	8.00	19.90	8.47	31.30	83.0	00610	00610
1530	21.0.	4.00	8.50	20.90	23.00	138.00	82.1	00510	00510
1600	24.0.	*****	*****	*****	*****	*****	****	****	****
1605	24.5.	13.00	8.00	19.40	20.90	208.00	80.7	00400	00400
1630	27.0.	18.00	7.50	15.90	32.20	244.00	78.3	00280	00280
1645	28.5.	*****	*****	*****	*****	*****	****	****	****
1700	30.0.	20.00	6.80	17.20	30.80	238.00	77.1	00130	00130
1734	334.	21.00	5.50	12.20	28.60	218.00	74.9	00190	00190

BAG-102  
DUAL OUTDOOR BAG DMAE SURROGATE RUN#2  
1979 APR 19

0600-0800 BAG # 11 FILLED WITH PURE AIR FROM CHAMBER SYSTEM  
BAG VOLUME APPROXIMATELY 44 CUBIC METERS

0745 BAG COVERED

0822 RH IS 14.6 AT 20 DEG C  
0925-0940 400 MICROLITERS (U-L) DMAE INJECTED AND MIXED  
1138 11.0 ML NO2 INJECTED AND MIXED  
1142 11.0 ML NO INJECTED AND MIXED

1344 BAG UNCOVERED

1715-1731 BAG EMPTY WITH A HIGH VOL RUNNING FREE (APP 65 CFM)

1150-1700 GAS PHASE DIRECT EXPOSURE TO MUTAGEN TESTING PLATES (1.6 LPM)  
TENAX GC-MS SAMPLES TAKEN

0855-0905 (0.67 L)  
1210-1220 (0.99 L)  
1325-1337 (0.59 L)  
1410-1420 (1.04 L)  
1508-1518 (1.06 L)  
1527-1557 (4.5 L)  
1600-1618 (0.87 L)  
1624-1649 (5.0 L)

\*MEASUREMENTS SO MARKED INCLUDE THE FOLLOWING UNITS AND FACTORS:

B-SCAT (METERS-1) X E+4  
CONDENSATION NUCLEI (PART/CUBIC CM) X E-3  
AEROSOL NUMBER (PART/CUBIC CM) X E-3  
AEROSOL SURFACE (U-METERS2/CUBIC CM) X E-2  
AEROSOL VOLUME (CUBIC U-METERS/CUBIC CM) X 1  
UV (CAL/CM2-MIN) X 1

T=0 AT 1200 PDT

TS DFG K AVERAGE  
UV AVERAGE 3.00 ± 2  
0.004

\* ASSIGNED INITIAL CONDITION

BAG-102  
DUAL OUTDOOR BAG CMAE SURROGATE RUN #2  
1979 APR 19

CLOCK TIME	ELAPSED TIME	OZONE PPM	OZONE PPM	NO PPM	NO2-CORR NOX-CORR PPM	PPM
	T (MIN)	BENDIX	BENDIX	BENDIX	BENDIX	BENDIX
820	-220.	*****	*****	0.011	0.0	0.0
825	-215.	0.007	0.007	0.011	0.0	0.0
1025	-95.	*****	*****	0.002	0.0	0.0
1040	-80.	0.016	0.016	0.002	0.0	0.0
1050	-70.	*****	*****	0.003	0.0	0.0
1110	-50.	*****	*****	0.003	0.0	0.0
1150	-10.	*****	*****	0.002	0.0	0.0
1200	0.	0.015	0.002	0.300	0.270	0.543
1220	20.	*****	*****	0.003	0.0	0.0
1230	30.	0.005	0.003	0.269	0.243	0.491
1250	50.	*****	*****	0.003	0.0	0.0
1305	65.	0.015	0.003	0.280	0.264	0.510
1320	80.	*****	*****	0.003	0.0	0.0
1335	95.	0.0	0.003	0.282	0.251	0.508
1400	120.	*****	0.006	0.281	0.233	0.500
1430	150.	*****	0.005	0.261	0.210	0.455
1500	180.	0.002	0.006	0.231	0.200	0.415
1505	185.	*****	*****	0.006	0.0	0.0
1535	215.	0.005	0.005	0.196	0.191	0.369
1600	240.	0.005	0.008	0.180	0.200	0.360
1630	270.	0.002	0.007	0.175	0.229	0.383
1700	300.	*****	*****	0.195	0.272	0.448
1701	301.	0.007	0.004	0.195	0.272	0.448

BAG-102  
DUAL OUTDOOR BAG DMAE SURROGATE RUN#2  
1979 APR 19

CLOCK ELAPSED TIME (MIN)	DMAE ppm	ACETALD ppm	ACETONE ppm	MEK ppm	ETHANE ppm	ETHENONE ppm	ACETYLENE ppm	PROPANE ppm	PROPENE ppm	1-C4 ppm	N-C4 ppm
820 -220.	0.0022	0.005	0.0025	0.0018	1.46	0.0040	0.0046	0.0017	0.0022	0.0004	0.001
825 -215.	***	***	***	***	***	***	***	***	***	***	***
1025 -95.	0.2082	***	***	***	***	***	***	***	***	***	***
1040 -80.	***	***	***	***	***	***	***	***	***	***	***
1050 -70.	0.4961	***	***	***	***	***	***	***	***	***	***
1110 -20.	0.5579	***	***	***	***	***	***	***	***	***	***
1150 -10.	0.4846	***	***	***	***	***	***	***	***	***	***
1200 0.	***	***	***	***	***	***	***	***	***	***	***
1220 20.	0.5136	***	***	***	***	***	***	***	***	***	***
1230 30.	***	***	***	***	***	***	***	***	***	***	***
1250 50.	0.5319	***	***	***	***	***	***	***	***	***	***
1305 65.	***	***	***	***	***	***	***	***	***	***	***
1320 80.	0.5683	***	***	***	***	***	***	***	***	***	***
1335 95.	***	***	***	***	***	***	***	***	***	***	***
1400 120.	0.5314	***	***	***	***	***	***	***	***	***	***
1430 150.	0.5080	***	***	***	***	***	***	***	***	***	***
1500 180.	***	***	***	***	***	***	***	***	***	***	***
1505 185.	0.4555	***	***	***	***	***	***	***	***	***	***
1535 215.	0.4555	***	***	***	***	***	***	***	***	***	***
1600 240.	0.4358	***	***	***	***	***	***	***	***	***	***
1630 270.	0.4166	***	***	***	***	***	***	***	***	***	***
1700 300.	0.3943	0.012	0.0041	***	1.48	0.0045	0.0049	0.0017	0.0023	0.0007	0.001
1701 301.	***	***	***	***	***	***	***	***	***	***	***

BAG-102  
 DUAL OUTGASS BAG DMAE SURROGATE RUN #2  
 1979 APR 19

CLOCK TIME	ELAPSED TIME	1-C4= PPM	1-C4= PPM	I-C5 PPM	N-C5 PPM	BENZENE PPM
820	-220.	0.0002	C.0001	0.0011	0.0003	0.0004
825	-215.	***	***	***	***	***
1025	-95.	***	***	***	***	***
1040	-80.	***	***	***	***	***
1050	-70.	***	***	***	***	***
1110	-50.	***	***	***	***	***
1150	-10.	***	***	***	***	***
1200	0.	***	***	***	***	***
1220	20.	***	***	***	***	***
1230	30.	***	***	***	***	***
1250	50.	***	***	***	***	***
1305	65.	***	***	***	***	***
1320	80.	***	***	***	***	***
1335	95.	***	***	***	***	***
1400	120.	***	***	***	***	***
1430	150.	***	***	***	***	***
1500	180.	***	***	***	***	***
1505	185.	***	***	***	***	***
1535	215.	***	***	***	***	***
1600	240.	***	***	***	***	***
1630	270.	***	***	***	***	***
1700	300.	0.0	0.0002	0.0012	0.0003	0.0007
1701	301.	***	***	***	***	***

BAG-102  
DUAL OUTDOOR BAG DMAE SURROGATE RUN #2  
1979 APR 19

CLOCK TIME T(MIN)	ELAPS'D TIME	B-SCAT	CONDENS.	AEROSL N	AEROSL S	AEROSL V	TS	DEG F	UV
		*	*	*	*	*	*	*	*
820	-220.	*****	*****	*****	*****	*****	*****	*****	*****
825	-215.	0.30	0.15	2.84	0.66	2.66	6.7	67.7	*****
1025	-95.	*****	*****	*****	*****	*****	*****	*****	*****
1040	-80.	0.40	19.50	44.00	10.30	26.60	*****	*****	*****
1050	-70.	*****	*****	*****	*****	*****	*****	*****	*****
1110	-50.	*****	*****	*****	*****	*****	*****	*****	*****
1150	-10.	*****	*****	*****	*****	*****	*****	*****	*****
1200	0.	1.40	40.00	91.40	3.40	11.40	81.2	*****	*****
1220	20.	*****	*****	*****	*****	*****	*****	*****	*****
1230	30.	1.50	31.00	85.00	31.00	100.20	05.7	*****	*****
1250	50.	*****	*****	*****	*****	*****	*****	*****	*****
1305	65.	1.60	27.00	66.20	23.90	101.00	82.1	*****	*****
1320	80.	*****	*****	*****	*****	*****	*****	*****	*****
1335	95.	1.60	23.00	60.40	28.30	100.00	*****	*****	*****
1400	120.	10.50	23.00	52.40	73.40	408.00	82.1	00460	*****
1430	150.	24.00	20.00	42.90	100.70	780.00	*****	00420	*****
1500	180.	37.50	19.00	40.60	95.00	680.00	U3.0	00410	*****
1505	185.	*****	*****	*****	*****	*****	*****	*****	*****
1535	215.	48.00	19.00	32.80	93.10	706.00	00380	00420	*****
1600	240.	51.00	18.00	31.10	89.50	698.00	81.2	00420	*****
1630	270.	55.00	13.00	25.40	79.70	632.00	*****	00270	*****
1700	300.	55.00	16.00	23.90	72.60	589.00	69.5	00230	*****
1701	301.								

BAG-103  
DUAL OUTDOOR DAG OMAE SURROGATE RUN #3  
1979 OCT 16

TIMES (PDT)  
0600-0750 BAG #11 FILLED WITH PURE AIR FROM CHAMBER SYSTEM

BAG VOLUME IS APPROXIMATELY 44 CUBIC METERS  
BAG COVERED  
0800 BAG COVERED  
0832 RH IS 30% AT 19 DEG C  
0905 5.5 ML NO INJECTED AND MIXED  
0908 2.0 ML NO.2 INJECTED AND MIXED  
0915 17.5 MICROLITER STU-LI 2.30WB INJECTED  
0922 540 ML SURROGATE J INJECTED  
0927 2.3 U-L TOLUENE, 2.0 U-L 2MEC-2, 6.7 U-L M-XYLENE INJECTED  
0935 BAG MIXED THOROUGHLY AND DIVIDED  
1000 12.24 U-L OMAE INJECTED INTO SIDE 1 AND MIXED  
(0.14 ppm in bag, calculated)  
1156 BAG UNCOVERED  
1648-1652 SIDE 1 EMPTIED WITH FREE-RUNNING HI-VOL SAMPLER TIGF (WASHED) FILTER  
TENAX GC-MS SAMPLES:

BAG UNDIVIDED: 0949-1014 (15.0 L)  
SIDE 1 1125-1142 (15.0 L)  
1412-1435 (15.0 L)  
1608-1633 (15.0 L)  
1106-1121 (15.0 L)  
1437-1501 (15.1 L)  
1634-1654 (15.0 L)

\*MEASUREMENTS SC MARKED INCLUDE THE FOLLOWING UNITS AND FACTORS:

$\beta$ -SCAT ((METERS-1) X E+4  
CONDENSATION NUCLEI (PART/CUBIC CM) X E-3  
AEROSOL NUMBER (PART/CUBIC CM) X E-3  
AEROSOL SURFACE (U-METERS2/CUBIC CM) X E-2  
AEROSOL VOLUME (CUBIC U-METERS/CUBIC CM) X 1  
UV (CAL/CM2-MIN) X 1

T=0 AT 1200 PDT

TS DEG K AVE PAGE  
UV AVERAGE 300.1  
UV 0.003

\* ASSIGNED INITIAL CONDITION

BAG-103 DUAL OUTDOOR DAG OMAE SURROGATE RUN #3  
1979 OCT 16

BAG-103  
DUAL OUTDOOR DAG DMAE SURROGATE RUN #3  
1979 OCT 16

CLOCK TIME	ELAPSED TIME (MIN)	DMAE	DMAE	PAN	ACETALD	ACETONE	MEK	METHANE
		PPM	PPM	PPM	PPM	PPM	PPM	PPM
SIDE 1	SIDE 2	SIDE 1	SIDE 2	SIDE 1	SIDE 2	SIDE 1	SIDE 2	SIDE 1
830	-210.	*****	*****	0.002	0.002	0.0004	0.0007	1.57
832	-208.	*****	*****	0.0	*****	*****	*****	*****
850	-190.	*****	*****	*****	*****	*****	*****	*****
936	-144.	*****	*****	0.0	*****	*****	*****	*****
945	-135.	*****	*****	*****	*****	*****	*****	1.76
952	-128.	*****	*****	0.0	*****	*****	*****	*****
1015	-105.	*****	*****	0.0	*****	*****	*****	*****
1028	-92.	*****	*****	0.0	*****	*****	*****	*****
1045	-75.	*****	*****	0.0	*****	*****	*****	*****
1051	-69.	*****	*****	0.0	*****	*****	*****	*****
1056	-64.	0.0726	*****	0.0	*****	*****	*****	1.75
1110	-50.	*****	*****	*****	*****	*****	*****	*****
1115	-45.	*****	*****	0.0	*****	*****	*****	*****
1118	-42.	0.0764	*****	0.0	*****	*****	*****	*****
1126	-34.	*****	*****	0.0	*****	*****	*****	*****
1139	-21.	0.0826	*****	*****	*****	*****	*****	*****
1145	-15.	*****	*****	*****	*****	*****	*****	*****
1200	0.	*****	*****	0.0	*****	*****	*****	*****
1214	14.	*****	*****	0.0	*****	*****	*****	*****
1230	30.	*****	*****	0.0	*****	*****	*****	*****
1237	37.	*****	*****	0.0	*****	*****	*****	*****
1300	60.	*****	*****	0.000	*****	*****	*****	*****
1306	66.	*****	*****	0.0	*****	*****	*****	*****
1314	74.	*****	*****	0.000	*****	*****	*****	*****
1315	75.	*****	*****	*****	*****	*****	*****	*****
1321	81.	0.0258	*****	*****	*****	*****	*****	*****
1330	90.	*****	*****	0.001	*****	*****	*****	*****
1340	100.	*****	*****	0.001	*****	*****	*****	*****
1345	105.	0.0226	*****	*****	*****	*****	*****	*****
1400	120.	*****	*****	0.001	*****	*****	*****	*****
1413	133.	0.0157	*****	*****	*****	*****	*****	*****
1414	134.	*****	*****	0.002	*****	*****	*****	*****
1430	150.	*****	*****	0.002	*****	*****	*****	*****
1438	158.	0.0116	*****	*****	*****	*****	*****	*****
1500	180.	*****	*****	0.003	*****	*****	*****	*****
1502	1d2.	*****	*****	*****	*****	*****	*****	*****
1507	187.	*****	*****	0.770	*****	0.0339	0.0062	1.71
1514	194.	*****	*****	0.003	*****	*****	*****	*****
1524	204.	*****	*****	0.006	*****	*****	*****	*****
1535	215.	*****	*****	0.003	*****	*****	*****	*****
1539	219.	0.0065	*****	0.006	*****	*****	*****	*****
1545	225.	*****	*****	*****	0.703	*****	0.0225	*****
1546	226.	*****	*****	0.006	*****	*****	*****	*****
1600	240.	*****	*****	0.003	*****	*****	*****	*****
1602	242.	0.0047	*****	*****	*****	*****	*****	*****
1609	249.	*****	*****	0.006	*****	*****	0.0048	*****
1615	255.	*****	*****	*****	0.720	*****	0.0036	*****
1635	275.	*****	*****	0.003	*****	*****	*****	*****
1639	279.	0.0015	*****	*****	*****	*****	0.0278	0.0060
1645	285.	*****	*****	*****	0.697	*****	*****	*****
1702	302.	*****	*****	*****	*****	*****	*****	1.73

BAG-103  
DUAL OUTDOOR DAG CMAC SURROGATE RUN #3  
1979 OCT 16

CLOCK ELAPSED	ETHANE	ETHENE	ACETYLEN	ACETYLEN	PROPANE	PROPENE
TIME (MIN)	PPM	PPM	PPM	PPM	PPM	PPM
0.30	-210.	*****	*****	SIDE 1	SIDE 2	SIDE 2
0.32	-208.	*****	*****	0.0038	0.0028	0.001
0.50	-190.	0.0579	*****	0.0038	0.0033	0.001
0.96	-144.	*****	*****	*****	*****	*****
0.95	-135.	0.1338	0.1338	0.0399	0.0383	0.013
0.952	-128.	*****	*****	*****	0.0430	0.0397
1.015	-105.	*****	*****	*****	0.0430	0.013
1.028	-92.	*****	*****	*****	*****	*****
1.048	-75.	*****	*****	*****	*****	*****
1.051	-69.	*****	*****	*****	*****	*****
1.056	-64.	*****	*****	*****	*****	*****
1.110	-59.	*****	0.1305	*****	0.0466	0.0410
1.115	-45.	*****	*****	0.0317	0.0466	0.0410
1.200	0.	*****	*****	*****	*****	*****
1.214	14.	*****	*****	0.0430	0.0460	0.0410
1.230	30.	*****	*****	*****	*****	*****
1.237	37.	*****	*****	*****	*****	*****
1.300	60.	*****	*****	*****	*****	*****
1.306	66.	*****	*****	*****	*****	*****
1.314	74.	*****	*****	*****	*****	*****
1.315	75.	*****	0.1360	*****	0.0453	0.0406
1.321	81.	*****	*****	*****	*****	0.0411
1.330	90.	*****	*****	*****	*****	*****
1.340	100.	*****	*****	*****	*****	*****
1.345	105.	*****	*****	*****	*****	*****
1.400	120.	*****	0.1352	*****	0.0442	0.0408
1.413	133.	*****	*****	*****	*****	*****
1.414	134.	*****	*****	*****	*****	*****
1.430	150.	*****	*****	*****	*****	*****
1.438	158.	*****	*****	*****	*****	*****
1.500	180.	*****	*****	*****	*****	*****
1.502	182.	*****	*****	*****	*****	*****
1.507	187.	*****	*****	*****	*****	*****
1.514	194.	*****	*****	*****	*****	*****
1.524	204.	*****	*****	*****	*****	*****
1.535	215.	*****	*****	*****	*****	*****
1.539	219.	*****	*****	*****	*****	*****
1.609	249.	*****	0.1290	*****	0.0311	0.0420
1.615	255.	0.1323	*****	0.0299	0.0442	0.0421
1.646	229.	*****	*****	*****	*****	*****
1.600	240.	*****	*****	*****	*****	*****
1.602	242.	*****	*****	*****	*****	*****
1.645	285.	*****	*****	*****	*****	*****
1.702	302.	*****	*****	*****	*****	*****

BAG-103  
DUAL OUTDOOR DAG DMAE SURROGATE RUN #3  
1979 OCT 16

CLOCK TIME	ELAPSED TIME (MIN)	I-C4	N-C4	I-C4	N-C4	I-C4=	I-C4=	T2-C4=	T2-C4=	I-C5
		PPM								
		SIDE 1	SIDE 2	SIDE 1						
830	-210.	0.0016	0.0016	0.001	0.0001	0.0001	0.0001	0.0008	0.0008	0.0008
832	-208.	*****	*****	*****	*****	*****	*****	*****	*****	*****
850	-190.	*****	*****	*****	*****	*****	*****	*****	*****	*****
936	-144.	*****	*****	*****	*****	*****	*****	*****	*****	*****
945	-135.	0.0017	0.0017	0.197	0.0003	0.0001	0.0001	0.0008	0.0008	0.0008
952	-128.	*****	*****	*****	*****	*****	*****	*****	*****	*****
1015	-105.	*****	*****	*****	*****	*****	*****	*****	*****	*****
1028	-92.	*****	*****	*****	*****	*****	*****	*****	*****	*****
1045	-75.	*****	*****	*****	*****	*****	*****	*****	*****	*****
1051	-69.	*****	*****	*****	*****	*****	*****	*****	*****	*****
1056	-64.	*****	*****	*****	*****	*****	*****	*****	*****	*****
1110	-50.	*****	*****	0.0017	0.200	*****	*****	0.0002	0.0007	0.0005
1115	-45.	*****	*****	*****	*****	*****	*****	*****	*****	*****
1118	-42.	*****	*****	*****	*****	*****	*****	*****	*****	*****
1126	-34..	*****	*****	*****	*****	*****	*****	*****	*****	*****
1139	-21..	*****	*****	*****	*****	*****	*****	*****	*****	*****
1145	-15..	0.0017	0.0017	0.202	0.0002	0.0002	0.0002	0.0005	0.0005	0.0005
1200	0..	*****	*****	*****	*****	*****	*****	*****	*****	*****
1214	14..	*****	*****	*****	*****	*****	*****	*****	*****	*****
1230	30..	*****	*****	0.0017	0.197	*****	*****	0.0001	0.0005	0.0008
1237	37..	*****	*****	*****	*****	*****	*****	*****	*****	*****
1300	60..	*****	*****	*****	*****	*****	*****	*****	*****	*****
1306	69..	*****	*****	*****	*****	*****	*****	*****	*****	*****
1314	74..	*****	*****	*****	*****	*****	*****	*****	*****	*****
1315	75..	0.0017	0.199	0.0002	0.0002	0.0001	0.0001	0.0004	0.0005	0.0006
1321	81..	*****	*****	*****	*****	*****	*****	*****	*****	*****
1330	90..	*****	*****	*****	*****	*****	*****	*****	*****	*****
1340	100..	*****	*****	*****	*****	*****	*****	*****	*****	*****
1345	105..	*****	*****	*****	*****	*****	*****	*****	*****	*****
1400	120..	*****	*****	0.0016	0.191	*****	*****	0.0001	0.0002	0.0006
1413	133..	*****	*****	*****	*****	*****	*****	*****	*****	*****
1414	134..	*****	*****	*****	*****	*****	*****	*****	*****	*****
1430	150..	*****	*****	*****	*****	*****	*****	*****	*****	*****
1438	158..	*****	*****	*****	*****	*****	*****	*****	*****	*****
1500	180..	*****	*****	*****	*****	*****	*****	*****	*****	*****
1502	182..	*****	*****	*****	*****	*****	*****	0.0002	0.0001	0.0004
1507	187..	0.0015	0.184	0.0002	0.183	0.0001	0.0001	0.0001	0.0	0.0004
1514	194..	*****	*****	*****	*****	*****	*****	*****	*****	*****
1520	204..	*****	*****	*****	*****	*****	*****	*****	*****	*****
1524	215..	*****	*****	*****	*****	*****	*****	*****	*****	*****
1535	219..	*****	*****	*****	*****	*****	*****	*****	*****	*****
1545	225..	*****	*****	0.0016	0.183	*****	*****	0.0002	0.0	0.0004
1546	226..	*****	*****	*****	*****	*****	*****	*****	*****	*****
1600	240..	*****	*****	*****	*****	*****	*****	0.0001	0.0001	0.0007
1602	242..	*****	*****	*****	*****	*****	*****	*****	*****	*****
1609	249..	*****	*****	*****	*****	*****	*****	*****	*****	*****
1615	255..	0.0017	0.182	0.0001	0.176	0.0001	0.0001	0.0002	0.0	0.0004
1635	275..	*****	*****	*****	*****	*****	*****	*****	*****	*****
1639	279..	*****	*****	*****	*****	*****	*****	*****	*****	*****
1645	285..	0.0016	0.176	0.0001	0.176	0.0001	0.0001	0.0001	0.0	0.0004
1702	302..	*****	*****	*****	*****	*****	*****	*****	*****	*****

BAG-103  
DUAL OUTDOOR DAG DMAE SURROGATE RUN #3  
1979 OCT 16

TIME	ELAPSED	CLOCK	C1S2-C4=	CIS2-C4=	N-C5	2-ME-C4=2	2-ME-C4=2	2,3-DMB	2,3-DMB	TOLUENE	TOLUENE	M-XYL
T (MIN)		SIDE 1	SIDE 2	SIDE 1	SIDE 2	SIDE 1	SIDE 2	SIDE 1	SIDE 2	SIDE 1	SIDE 2	SIDE 1
		SIDE 1	SIDE 2	SIDE 1	SIDE 2	SIDE 1	SIDE 2	SIDE 1	SIDE 2	SIDE 1	SIDE 2	SIDE 1
0.30	-21.0.	*****	*****	0.0003	0.0028	*****	*****	*****	*****	0.000	0.000	*****
0.32	-20.6.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
0.50	-19.0.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
0.36	-14.4.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
0.45	-13.5.	0.0150	0.0150	0.0005	0.0108	0.0108	0.0108	0.0102	0.0102	0.015	0.015	0.0378
0.52	-12.8.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1.15	-10.5.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1.20	-9.2.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1.45	-7.5.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1.51	-6.3.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1.56	-6.4.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1.10	-5.0.	*****	*****	0.0148	0.0003	*****	*****	*****	*****	0.015	0.015	0.0376
1.15	-4.5.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1.18	-4.2.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1.26	-3.4.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1.39	-2.1.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1.45	-1.5.	0.0149	0.0002	*****	*****	0.0099	*****	*****	*****	0.015	0.015	0.0382
1.20	0.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1.14	1.4.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1.20	3.0.	*****	*****	0.0116	0.0003	*****	*****	*****	*****	0.015	0.015	0.0340
1.27	3.7.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1.00	6.0.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1.06	6.6.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1.14	7.4.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1.20	7.5.	0.0088	0.0002	*****	*****	0.0025	*****	*****	*****	0.015	0.015	0.0340
1.21	8.1.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1.30	9.0.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1.40	10.0.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1.45	10.5.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1.50	11.5.	0.0036	0.0002	*****	*****	0.0002	*****	*****	*****	0.015	0.015	0.0250
1.60	12.0.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1.13	13.3.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1.14	13.4.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1.30	15.0.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1.38	15.9.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1.00	18.0.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1.02	18.2.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1.07	18.7.	0.0002	0.0002	*****	*****	0.0002	*****	*****	*****	0.013	0.013	0.0203
1.14	19.4.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1.24	20.4.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1.00	24.0.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1.35	21.5.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1.39	21.9.	*****	*****	*****	*****	*****	*****	*****	*****	0.011	0.011	0.0191
1.45	22.5.	*****	*****	0.0003	0.0002	*****	*****	*****	*****	0.075	0.075	0.159
1.46	22.9.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1.00	24.0.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1.02	24.2.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1.07	24.9.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1.14	19.4.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1.30	25.5.	0.0	0.0	0.0001	0.0001	*****	*****	*****	*****	*****	*****	*****
1.35	27.5.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1.39	27.9.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1.45	28.5.	0.0	0.0	0.0002	0.0002	*****	*****	*****	*****	0.012	0.012	0.0177
1.02	30.2.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****

BAG-103  
DUAL OUTDOOR LAG DMAE SURROGATE RUN #3  
1979 OCT 16

CLOCK TIME (MIN)	ELAPSED	B-SCAT	CONDENS.	AEROSL N	AEROSL S	AEROSL V	TS	TS	DEG F	DEG F	UV
0.30	-210.	***	***	***	***	***	***	***	***	***	***
0.32	-206.	***	***	0.50	***	0.0	***	1.36	0.50	0.94	65.9
0.50	-190.	***	***	***	***	***	***	***	***	***	***
0.36	-144.	***	***	0.50	***	0.20	***	0.95	0.49	2.21	***
0.45	-135.	***	***	***	***	***	***	***	***	***	***
0.52	-129.	0.50	***	0.20	***	1.23	***	0.67	1.66	***	***
1.015	-105.	***	0.60	***	0.40	***	1.38	0.42	1.97	***	71.3
1.028	-92.	0.60	***	0.50	***	1.58	***	0.47	1.70	***	***
1.045	-75.	***	0.60	***	0.60	***	1.78	0.55	2.18	***	74.9
1.051	-69.	***	***	***	***	***	***	***	***	***	***
1.056	-64.	0.50	***	0.50	***	2.06	***	1.02	0.50	***	***
1.110	-50.	***	***	***	***	***	***	***	0.96	3.77	***
1.115	-45.	***	0.60	***	0.60	***	1.74	***	0.55	***	80.3
1.118	-42.	***	***	***	***	***	***	***	***	***	***
1.126	-34.	0.60	***	0.50	***	1.87	***	0.66	1.09	***	***
1.139	-21.	***	***	***	***	***	***	***	***	***	***
1.145	-15.	***	***	***	***	***	***	***	***	***	***
1.200	0.	***	***	0.70	***	0.60	***	1.85	0.46	1.86	***
1.214	14.	0.70	***	3.80	0.00	90.09	***	15.70	34.70	***	0.3
1.230	30.	***	***	0.70	***	0.20	***	2.13	0.57	2.52	***
1.237	37.	1.00	***	3.40	0.00	82.70	***	27.70	72.00	***	82.1
1.300	60.	***	0.60	***	0.80	***	0.99	0.54	2.54	***	0.0410
1.306	66.	***	***	***	***	***	***	***	***	***	***
1.314	74.	2.60	***	30.00	***	72.60	***	50.60	188.00	***	82.1
1.315	75.	***	***	***	***	***	***	***	***	***	***
1.321	81.	***	***	***	***	***	***	***	***	***	***
1.330	90.	***	0.60	***	1.00	***	1.42	0.48	2.15	***	78.5
1.340	100.	7.10	***	26.00	***	68.30	***	73.00	343.00	***	0.0350
1.345	105.	***	***	***	***	***	***	***	***	***	***
1.400	120.	***	0.70	***	0.90	***	1.52	0.59	3.24	***	0.0380
1.410	133.	***	***	***	***	***	***	***	***	***	***
1.414	134.	15.70	***	23.00	***	59.10	***	90.40	506.00	***	0.3
1.430	150.	***	0.70	***	1.60	***	0.95	0.51	2.53	***	80.3
1.438	158.	***	***	***	***	***	***	***	***	***	***
1.500	180.	15.40	***	19.00	***	34.70	***	80.90	404.00	***	0.9
1.502	182.	***	***	***	***	***	***	1.12	0.55	2.38	***
1.507	187.	***	***	***	***	***	***	***	***	***	***
1.514	194.	0.80	***	0.80	***	0.60	***	0.71	0.67	4.23	***
1.524	204.	13.00	***	17.70	***	38.00	***	64.60	383.00	***	82.1
1.535	215.	***	***	0.60	***	1.10	***	1.12	0.55	2.38	***
1.539	219.	9.00	***	13.20	***	29.60	***	47.80	211.00	***	0.3
1.545	225.	16.15	***	16.00	***	34.10	***	56.80	336.00	***	0.7
1.546	226.	11.00	***	16.00	***	1.10	***	1.61	0.77	3.44	***
1.600	240.	***	0.60	***	1.10	***	2.19	0.76	3.12	***	78.5
1.602	242.	***	***	***	***	***	***	***	***	***	0.0260
1.609	249.	9.00	***	13.20	***	29.60	***	47.80	211.00	***	0.3
1.615	255.	16.15	***	16.00	***	34.10	***	56.80	336.00	***	0.7
1.635	275.	11.00	***	16.00	***	1.10	***	2.19	0.76	3.12	***
1.639	279.	***	***	***	***	***	***	***	***	***	***
1.645	285.	9.00	***	13.20	***	29.60	***	47.80	211.00	***	0.3
1.702	302.	***	***	***	***	***	***	***	***	***	***

BAG-10<sup>4</sup>  
OMAE SURROGATE RUN #4  
1973 OCT 23

TIME (PDT)  
0600-0738 BAG #11 FILLED WITH PURE AIR FROM CHAMBER SYSTEM  
BAG VOLUME IS APPROXIMATELY .33 CUBIC METERS  
0800 BAG COVERED  
0d30 PH 1.5 25% AT T=19 DEG C  
0841 2.6 ML NO<sub>2</sub> INJECTED AND MIXED  
0843 7.3 ML NO<sub>2</sub> INJECTED AND MIXED  
0945 500 ML SURROGATE J INJECTED  
0900 13.1 MICROLITERSULJ 2,3DMB, 1.7 U-L TOLUENE, 1.5 U-L 2MEC4-2,  
5.0 U-L M-XYLENE INJECTED  
0910 BAG MIXED THOROUGHLY AND DIVIDED  
0925 3.5 U-L OMAE INJECTED INTO SIDE 1  
0925 (0.05 ppm IN BAG, CALCULATED)  
1140 BAG UNCOVERED  
1703-1706 SIDE ONE EMPTIED WITH FREE RUNNING HI VOL SAMPLER  
USED SOLVENT-WASHED TIGE FILTER #174  
UPPER LIMIT OF HNO<sub>3</sub> IS 0.010 ppm USING NOX ANALYZER WITH  
AND WITHOUT NYLCN SCRUBBER ]

\*MEASUREMENTS SO MARKED INCLUDE THE FOLLOWING UNITS AND FACTORS:  
B-SCAT (METERS-1) X E+4  
CONDENSATION NUCLEI (PART/CUBIC CM) X E-3  
AEROSOL NUMBER (PART/CUBIC CM) X E-3  
AEROSOL SURFACE (.U-METERS<sup>2</sup>/CUBIC CM) X E-2  
AEROSOL VOLUME (CUBIC U-METERS/CUBIC CM) X 1  
UV (CAL/CM<sup>2</sup>-MIN) X 1

T=0 AT 1140 PDT

TS DEG K AVERAGE 297.6  
UV AVERAGE 0.003

\* ASSIGNED INITIAL CONDITION

BAG-104  
DMAE SURROGATE RUN #4  
1979 OCT 23

CLOCK TIME	ELAPSED TIME (MIN)	OZONE PPM	OZONE PPM	OZONE PPM	OZONE PPM	NO PPM	NO PPM	NO2-CORR PPM	NO2-CORR PPM	NO2-CORR PPM	NO2-CORR PPM	NOX-CORR PPM
949	-202.	0.003	0.003	0.003	0.003	0.010	0.010	0.001	0.001	0.001	0.001	0.011
950	-200.	***	***	***	***	***	***	***	***	***	***	***
951	-185.	***	***	***	***	***	***	***	***	***	***	***
952	-168.	0.003	0.003	0.003	0.003	0.003	0.003	0.094	0.094	0.094	0.094	0.260
953	-136.	***	***	***	***	0.0	0.0	0.169	0.169	0.169	0.169	0.260
954	-130.	***	***	***	***	***	***	***	***	***	***	***
955	-111.	0.004	0.004	0.004	0.004	0.004	0.004	0.092	0.092	0.092	0.092	0.253
956	-109.	***	***	***	***	***	***	***	***	***	***	***
957	-102.	***	***	***	***	0.004	0.004	0.161	0.161	0.161	0.161	0.255
958	-90.	***	***	***	***	0.004	0.004	0.093	0.093	0.093	0.093	0.255
959	-89.	***	***	***	***	0.003	0.003	0.169	0.169	0.169	0.169	0.260
960	-88.	***	***	***	***	0.0	0.0	0.164	0.164	0.164	0.164	0.260
961	-85.	0.003	0.003	0.003	0.003	0.0	0.0	0.161	0.161	0.161	0.161	0.255
962	-75.	***	***	***	***	0.004	0.004	0.0	0.0	0.0	0.0	0.250
963	-70.	***	***	***	***	0.004	0.004	0.161	0.161	0.161	0.161	0.255
964	-55.	0.002	0.002	0.002	0.002	0.0	0.0	0.167	0.167	0.167	0.167	0.257
965	-50.	***	***	***	***	0.004	0.004	0.094	0.094	0.094	0.094	0.255
966	-45.	***	***	***	***	0.003	0.003	0.161	0.161	0.161	0.161	0.255
967	-43.	***	***	***	***	0.004	0.004	0.161	0.161	0.161	0.161	0.255
968	-25.	0.0	0.0	0.0	0.0	0.004	0.004	0.165	0.165	0.165	0.165	0.258
969	-24.	***	***	***	***	0.002	0.002	0.167	0.167	0.167	0.167	0.258
970	-16.	***	***	***	***	0.004	0.004	0.0	0.0	0.0	0.0	0.255
971	0.	***	***	***	***	0.004	0.004	0.163	0.163	0.163	0.163	0.255
972	45.	0.010	0.010	0.010	0.010	0.008	0.008	0.099	0.099	0.099	0.099	0.251
973	5.	***	***	***	***	0.004	0.004	0.161	0.161	0.161	0.161	0.250
974	15.	***	***	***	***	0.011	0.011	0.010	0.010	0.010	0.010	0.249
975	35.	0.010	0.010	0.010	0.010	0.001	0.001	0.126	0.126	0.126	0.126	0.243
976	36.	***	***	***	***	0.004	0.004	0.098	0.098	0.098	0.098	0.255
977	49.	***	***	***	***	0.010	0.010	0.163	0.163	0.163	0.163	0.255
978	110.	***	***	***	***	0.016	0.016	0.120	0.120	0.120	0.120	0.243
979	64.	***	***	***	***	0.024	0.024	0.024	0.024	0.024	0.024	0.243
980	125.	0.013	0.013	0.013	0.013	0.010	0.010	0.150	0.150	0.150	0.150	0.249
981	66.	***	***	***	***	0.024	0.024	0.010	0.010	0.010	0.010	0.249
982	80.	***	***	***	***	0.025	0.025	0.009	0.009	0.009	0.009	0.243
983	95.	0.026	0.026	0.026	0.026	0.012	0.012	0.160	0.160	0.160	0.160	0.234
984	110.	***	***	***	***	0.020	0.020	0.016	0.016	0.016	0.016	0.232
985	125.	0.024	0.024	0.024	0.024	0.024	0.024	0.167	0.167	0.167	0.167	0.226
986	136.	0.024	0.024	0.024	0.024	0.016	0.016	0.161	0.161	0.161	0.161	0.229
987	155.	0.025	0.025	0.025	0.025	0.024	0.024	0.168	0.168	0.168	0.168	0.220
988	166.	***	***	***	***	0.020	0.020	0.015	0.015	0.015	0.015	0.219
989	170.	***	***	***	***	0.016	0.016	0.016	0.016	0.016	0.016	0.219
990	172.	***	***	***	***	0.024	0.024	0.024	0.024	0.024	0.024	0.219
991	172.	***	***	***	***	0.030	0.030	0.032	0.032	0.032	0.032	0.219
992	185.	0.032	0.032	0.032	0.032	0.024	0.024	0.035	0.035	0.035	0.035	0.219
993	195.	***	***	***	***	0.015	0.015	0.018	0.018	0.018	0.018	0.218
994	200.	***	***	***	***	0.026	0.026	0.028	0.028	0.028	0.028	0.208
995	215.	0.045	0.045	0.045	0.045	0.049	0.049	0.036	0.036	0.036	0.036	0.193
996	217.	***	***	***	***	0.030	0.030	0.031	0.031	0.031	0.031	0.193
997	227.	***	***	***	***	0.029	0.029	0.029	0.029	0.029	0.029	0.193
998	229.	***	***	***	***	0.024	0.024	0.024	0.024	0.024	0.024	0.193
999	245.	0.038	0.038	0.038	0.038	0.015	0.015	0.021	0.021	0.021	0.021	0.193
1000	260.	***	***	***	***	0.026	0.026	0.031	0.031	0.031	0.031	0.193
1001	275.	0.045	0.045	0.045	0.045	0.049	0.049	0.021	0.021	0.021	0.021	0.193
1002	291.	***	***	***	***	0.030	0.030	0.032	0.032	0.032	0.032	0.193
1003	304.	0.046	0.046	0.046	0.046	0.048	0.048	0.018	0.018	0.018	0.018	0.193
1004	305.	***	***	***	***	0.030	0.030	0.031	0.031	0.031	0.031	0.193
1005	310.	***	***	***	***	0.029	0.029	0.029	0.029	0.029	0.029	0.193

BAG-104  
DMAE SURROGATE RUN #4  
1979 OCT 23

CLOCK	FLAPSFD	DMAE	CMAE	PAN	PAN	ACETALD	ACETALD	ACETONE	ACETONE	MEK	MEK	METHANE	METHANE
TIME	(MIN)	SIDE 1	SIDE 2	SIDE 1	SIDE 2	SIDE 1	SIDE 2	SIDE 1	SIDE 2	SIDE 1	SIDE 2	SIDE 1	SIDE 2
918	-202.	*****	*****	0.0	*****	0.003	0.003	0.0003	0.0003	*****	*****	*****	*****
920	-200.	*****	*****	0.0	*****	0.003	0.003	0.0003	0.0003	*****	*****	*****	*****
835	-185.	0.0	0.0	0.0	*****	0.0	0.0	0.0003	0.0003	*****	*****	*****	*****
912	-148.	*****	*****	0.0	*****	0.0	0.0	0.0003	0.0003	*****	*****	*****	*****
924	-136.	*****	*****	0.0	*****	0.0	0.0	0.0003	0.0003	*****	*****	*****	*****
930	-130.	*****	*****	0.0	*****	0.0	0.0	0.0003	0.0003	*****	*****	*****	*****
949	-111.	*****	*****	0.0	*****	0.0	0.0	0.0003	0.0003	*****	*****	*****	*****
951	-109.	0.0109	*****	0.0	*****	0.0	0.0	0.0003	0.0003	*****	*****	*****	*****
958	-102.	*****	*****	0.0	*****	0.0	0.0	0.0003	0.0003	*****	*****	*****	*****
1010	-90.	*****	*****	0.0	*****	0.0	0.0	0.0003	0.0003	*****	*****	*****	*****
1011	-89.	*****	*****	0.0	*****	0.0	0.0	0.0003	0.0003	*****	*****	*****	*****
1012	-88.	0.0125	*****	0.0	*****	0.0	0.0	0.0003	0.0003	*****	*****	*****	*****
1015	-85.	*****	*****	0.0	*****	0.0	0.0	0.0003	0.0003	*****	*****	*****	*****
1025	-75.	*****	*****	0.0	*****	0.0	0.0	0.0003	0.0003	*****	*****	*****	*****
1030	-70.	0.0131	*****	0.0	*****	0.0	0.0	0.0003	0.0003	*****	*****	*****	*****
1045	-55.	*****	*****	0.0	*****	0.0	0.0	0.0003	0.0003	*****	*****	*****	*****
1050	-50.	0.0160	*****	0.0	*****	0.0	0.0	0.0003	0.0003	*****	*****	*****	*****
1055	-45.	*****	*****	0.0	*****	0.0	0.0	0.0003	0.0003	*****	*****	*****	*****
1057	-43.	*****	*****	0.0	*****	0.0	0.0	0.0003	0.0003	*****	*****	*****	*****
1115	-25.	*****	*****	0.0	*****	0.0	0.0	0.0003	0.0003	*****	*****	*****	*****
1116	-24.	0.0111	*****	0.0	*****	0.0	0.0	0.0003	0.0003	*****	*****	*****	*****
1122	-14.	*****	*****	0.0	*****	0.0	0.0	0.0003	0.0003	*****	*****	*****	*****
1140	0.	*****	*****	0.0	*****	0.0	0.0	0.0003	0.0003	*****	*****	*****	*****
1145	5.	*****	*****	0.0	*****	0.0	0.0	0.0003	0.0003	*****	*****	*****	*****
1155	15.	*****	*****	0.0	*****	0.0	0.0	0.0003	0.0003	*****	*****	*****	*****
1215	35.	*****	*****	0.0	*****	0.0	0.0	0.0003	0.0003	*****	*****	*****	*****
1216	36.	0.0047	*****	0.0	*****	0.0	0.0	0.0003	0.0003	*****	*****	*****	*****
1229	49.	*****	*****	0.0	*****	0.0	0.0	0.0003	0.0003	*****	*****	*****	*****
1244	64.	0.0055	*****	0.0	*****	0.0	0.0	0.0003	0.0003	*****	*****	*****	*****
1246	66.	*****	*****	0.0	*****	0.0	0.0	0.0003	0.0003	*****	*****	*****	*****
1300	80.	*****	*****	0.0	*****	0.0	0.0	0.0003	0.0003	*****	*****	*****	*****
1315	93.	0.0042	*****	0.0	*****	0.0	0.0	0.0003	0.0003	*****	*****	*****	*****
1330	110.	0.0038	*****	0.0	*****	0.0	0.0	0.0003	0.0003	*****	*****	*****	*****
1345	125.	0.0010	*****	0.0	*****	0.0	0.0	0.0003	0.0003	*****	*****	*****	*****
1356	136.	0.0026	*****	0.0	*****	0.0	0.0	0.0003	0.0003	*****	*****	*****	*****
1415	155.	0.0026	*****	0.0	*****	0.000	0.000	0.0003	0.0003	*****	*****	*****	*****
1426	166.	*****	*****	0.0	*****	0.000	0.000	0.0003	0.0003	*****	*****	*****	*****
1430	170.	0.0011	*****	0.0	*****	0.000	0.000	0.0003	0.0003	*****	*****	*****	*****
1432	172.	0.0008	*****	0.0	*****	0.000	0.000	0.0003	0.0003	*****	*****	*****	*****
1445	185.	*****	*****	0.0	*****	0.000	0.000	0.0003	0.0003	*****	*****	*****	*****
1455	195.	*****	*****	0.0	*****	0.000	0.000	0.0003	0.0003	*****	*****	*****	*****
1500	200.	0.0011	*****	0.0	*****	0.000	0.000	0.0003	0.0003	*****	*****	*****	*****
1515	215.	*****	*****	0.0	*****	0.000	0.000	0.0003	0.0003	*****	*****	*****	*****
1527	227.	*****	*****	0.0	*****	0.000	0.000	0.0003	0.0003	*****	*****	*****	*****
1529	229.	0.002	*****	0.0	*****	0.000	0.000	0.0003	0.0003	*****	*****	*****	*****
1545	245.	*****	*****	0.0	*****	0.000	0.000	0.0003	0.0003	*****	*****	*****	*****
1600	260.	0.003	*****	0.0	*****	0.000	0.000	0.0003	0.0003	*****	*****	*****	*****
1615	275.	*****	*****	0.0	*****	0.001	0.001	0.0003	0.0003	*****	*****	*****	*****
1631	291.	*****	*****	0.0	*****	0.001	0.001	0.0003	0.0003	*****	*****	*****	*****
1644	304.	*****	*****	0.0	*****	0.017	0.017	0.0003	0.0003	*****	*****	*****	*****
1645	305.	C.0001	*****	0.0	*****	0.027	0.027	0.0003	0.0003	*****	*****	*****	*****
1650	310.	*****	*****	0.0	*****	0.0175	0.0175	0.0003	0.0003	*****	*****	*****	*****

CLOCK	ELAPSED TIME (MIN)	TIME	PPM	ETHANE	ETHENE	PPM	SIDE 1	SIDE 2	PROPENE		
									DMS-1	DMS-2	SIDE 1
918	-202.	818	0.0106	0.0106	0.0066	0.0066	0.0066	0.0066	0.0025	0.0025	0.001
820	-200.	912	0.0102	0.0102	0.0062	0.0062	0.0062	0.0062	0.0025	0.0025	0.001
835	-185.	914	0.0100	0.0100	0.0060	0.0060	0.0060	0.0060	0.0025	0.0025	0.001
912	-148.	924	0.0098	0.0098	0.0058	0.0058	0.0058	0.0058	0.0025	0.0025	0.001
924	-136.	930	0.0097	0.0097	0.0057	0.0057	0.0057	0.0057	0.0025	0.0025	0.001
930	-130.	949	0.0096	0.0096	0.0056	0.0056	0.0056	0.0056	0.0025	0.0025	0.001
949	-111.	951	0.0095	0.0095	0.0055	0.0055	0.0055	0.0055	0.0025	0.0025	0.001
951	-109.	1010	0.0094	0.0094	0.0054	0.0054	0.0054	0.0054	0.0025	0.0025	0.001
1025	-75.	1030	0.0086	0.0086	0.0049	0.0049	0.0049	0.0049	0.0025	0.0025	0.001
1030	-70.	1045	0.0083	0.0083	0.0048	0.0048	0.0048	0.0048	0.0025	0.0025	0.001
1045	-55.	1050	0.0081	0.0081	0.0047	0.0047	0.0047	0.0047	0.0025	0.0025	0.001
1050	-50.	1055	0.0080	0.0080	0.0046	0.0046	0.0046	0.0046	0.0025	0.0025	0.001
1055	-45.	1057	0.0079	0.0079	0.0045	0.0045	0.0045	0.0045	0.0025	0.0025	0.001
1057	-43.	1115	0.0078	0.0078	0.0044	0.0044	0.0044	0.0044	0.0025	0.0025	0.001
1115	-25.	1122	0.0077	0.0077	0.0043	0.0043	0.0043	0.0043	0.0025	0.0025	0.001
1122	-18.	1140	0.	0.	0.	0.	0.	0.	0.0025	0.0025	0.001
1140	0.	1145	0.	0.	0.	0.	0.	0.	0.0025	0.0025	0.001
1145	0.	1155	0.	0.	0.	0.	0.	0.	0.0025	0.0025	0.001
1155	1.5.	1215	0.00816	0.00816	0.00408	0.00408	0.00408	0.00408	0.0025	0.0025	0.001
1215	3.5.	1216	0.00816	0.00816	0.00408	0.00408	0.00408	0.00408	0.0025	0.0025	0.001
1216	36.	1229	0.00816	0.00816	0.00408	0.00408	0.00408	0.00408	0.0025	0.0025	0.001
1229	49.	1244	0.00805	0.00805	0.00407	0.00407	0.00407	0.00407	0.0025	0.0025	0.001
1244	64.	1246	0.00805	0.00805	0.00407	0.00407	0.00407	0.00407	0.0025	0.0025	0.001
1246	66.	1300	0.00804	0.00804	0.00408	0.00408	0.00408	0.00408	0.0025	0.0025	0.001
1300	80.	1315	0.00804	0.00804	0.00408	0.00408	0.00408	0.00408	0.0025	0.0025	0.001
1315	95.	1330	0.00804	0.00804	0.00408	0.00408	0.00408	0.00408	0.0025	0.0025	0.001
1330	110.	1345	0.00805	0.00805	0.00408	0.00408	0.00408	0.00408	0.0025	0.0025	0.001
1345	125.	1356	0.00804	0.00804	0.00408	0.00408	0.00408	0.00408	0.0025	0.0025	0.001
1356	136.	1415	0.00804	0.00804	0.00408	0.00408	0.00408	0.00408	0.0025	0.0025	0.001
1415	155.	1426	0.00804	0.00804	0.00408	0.00408	0.00408	0.00408	0.0025	0.0025	0.001
1426	166.	1430	0.00802	0.00802	0.00406	0.00406	0.00406	0.00406	0.0025	0.0025	0.001
1430	170.	1432	0.00802	0.00802	0.00406	0.00406	0.00406	0.00406	0.0025	0.0025	0.001
1432	172.	1445	0.00802	0.00802	0.00406	0.00406	0.00406	0.00406	0.0025	0.0025	0.001
1445	185.	1455	0.00802	0.00802	0.00406	0.00406	0.00406	0.00406	0.0025	0.0025	0.001
1455	195.	1500	0.00802	0.00802	0.00406	0.00406	0.00406	0.00406	0.0025	0.0025	0.001
1500	200.	1515	0.00802	0.00802	0.00406	0.00406	0.00406	0.00406	0.0025	0.0025	0.001
1515	215.	1527	0.00802	0.00802	0.00406	0.00406	0.00406	0.00406	0.0025	0.0025	0.001
1527	227.	1549	0.00802	0.00802	0.00406	0.00406	0.00406	0.00406	0.0025	0.0025	0.001
1549	229.	1555	0.00802	0.00802	0.00406	0.00406	0.00406	0.00406	0.0025	0.0025	0.001
1555	230.	1644	0.00802	0.00802	0.00406	0.00406	0.00406	0.00406	0.0025	0.0025	0.001
1644	249.	1645	0.00802	0.00802	0.00406	0.00406	0.00406	0.00406	0.0025	0.0025	0.001
1645	250.	1650	0.00802	0.00802	0.00406	0.00406	0.00406	0.00406	0.0025	0.0025	0.001

BAG-104  
OMAE SURROGATE RUN #4  
1979 OCT 23

CLOCK	FLAPSED	TIME	TMINI	I-C4	N-C4	I-C4	N-C4	I-C4=	T2-C4=	I-C5
				PPM						
910	-202.	0.0013	0.0013	SIDE 1	SIDE 2	SIDE 1	SIDE 2	SIDE 1	SIDE 2	SIDE 1
020	-200.	0.0013	0.0013	*****#	*****#	*****#	*****#	*****#	*****#	*****#
935	-105.	0.0013	0.0013	*****#	*****#	*****#	*****#	*****#	*****#	*****#
912	-148.	0.0013	0.0013	*****#	*****#	*****#	*****#	*****#	*****#	*****#
924	-130.	0.0013	0.0013	*****#	*****#	*****#	*****#	*****#	*****#	*****#
930	-130.	0.0012	0.0012	*****#	*****#	*****#	*****#	*****#	*****#	*****#
249	-111.	0.0012	0.0012	*****#	*****#	*****#	*****#	*****#	*****#	*****#
951	-109.	0.0012	0.0012	*****#	*****#	*****#	*****#	*****#	*****#	*****#
958	-102.	0.0014	0.0014	*****#	*****#	*****#	*****#	*****#	*****#	*****#
1010	-90.	0.0014	0.0014	*****#	*****#	*****#	*****#	*****#	*****#	*****#
1011	-89.	0.0014	0.0014	*****#	*****#	*****#	*****#	*****#	*****#	*****#
1012	-83.	0.0014	0.0014	*****#	*****#	*****#	*****#	*****#	*****#	*****#
1015	-85.	0.0014	0.0014	*****#	*****#	*****#	*****#	*****#	*****#	*****#
1025	-75.	0.0013	0.0013	*****#	*****#	*****#	*****#	*****#	*****#	*****#
1030	-70.	0.0014	0.0014	*****#	*****#	*****#	*****#	*****#	*****#	*****#
1045	-55.	0.0014	0.0014	*****#	*****#	*****#	*****#	*****#	*****#	*****#
1050	-50.	0.0014	0.0014	*****#	*****#	*****#	*****#	*****#	*****#	*****#
1055	-45.	0.0013	0.0013	*****#	*****#	*****#	*****#	*****#	*****#	*****#
1057	-43.	0.0013	0.0013	*****#	*****#	*****#	*****#	*****#	*****#	*****#
1115	-25.	0.0014	0.0014	*****#	*****#	*****#	*****#	*****#	*****#	*****#
1116	-24.	0.0014	0.0014	*****#	*****#	*****#	*****#	*****#	*****#	*****#
1122	-18.	0.0014	0.0014	*****#	*****#	*****#	*****#	*****#	*****#	*****#
1140	0.	0.0014	0.0014	*****#	*****#	*****#	*****#	*****#	*****#	*****#
1145	5.	0.0014	0.0014	*****#	*****#	*****#	*****#	*****#	*****#	*****#
1155	15.	0.0014	0.0014	*****#	*****#	*****#	*****#	*****#	*****#	*****#
1215	35.	0.0013	0.0013	*****#	*****#	*****#	*****#	*****#	*****#	*****#
1216	36.	0.0013	0.0013	*****#	*****#	*****#	*****#	*****#	*****#	*****#
1229	49.	0.0013	0.0013	*****#	*****#	*****#	*****#	*****#	*****#	*****#
1244	64.	0.0013	0.0013	*****#	*****#	*****#	*****#	*****#	*****#	*****#
1246	66.	0.0013	0.0013	*****#	*****#	*****#	*****#	*****#	*****#	*****#
1300	80.	0.0013	0.0013	*****#	*****#	*****#	*****#	*****#	*****#	*****#
1315	95.	0.0013	0.0013	*****#	*****#	*****#	*****#	*****#	*****#	*****#
1330	110.	0.0013	0.0013	*****#	*****#	*****#	*****#	*****#	*****#	*****#
1345	125.	0.0013	0.0013	*****#	*****#	*****#	*****#	*****#	*****#	*****#
1356	136.	0.0013	0.0013	*****#	*****#	*****#	*****#	*****#	*****#	*****#
1415	155.	0.0013	0.0013	*****#	*****#	*****#	*****#	*****#	*****#	*****#
1426	166.	0.0013	0.0013	*****#	*****#	*****#	*****#	*****#	*****#	*****#
1430	170.	0.0013	0.0013	*****#	*****#	*****#	*****#	*****#	*****#	*****#
1432	172.	0.0013	0.0013	*****#	*****#	*****#	*****#	*****#	*****#	*****#
1445	195.	0.0013	0.0013	*****#	*****#	*****#	*****#	*****#	*****#	*****#
1455	245.	0.0013	0.0013	*****#	*****#	*****#	*****#	*****#	*****#	*****#
1500	200.	0.0013	0.0013	*****#	*****#	*****#	*****#	*****#	*****#	*****#
1615	215.	0.0013	0.0013	*****#	*****#	*****#	*****#	*****#	*****#	*****#
1631	291.	0.0013	0.0013	*****#	*****#	*****#	*****#	*****#	*****#	*****#
1644	304.	0.0013	0.0013	*****#	*****#	*****#	*****#	*****#	*****#	*****#
1645	305.	0.0013	0.0013	*****#	*****#	*****#	*****#	*****#	*****#	*****#
1650	310.	0.0013	0.0013	*****#	*****#	*****#	*****#	*****#	*****#	*****#

BAG-104  
DMAE SURROGATE RUN #4  
1979 OCT 23

CLOCK	ELAPSED	TIME	TMIN	CIS2-C4=	CIS2-C4=	N-C5	2ME-C4=2	2ME-C4=2	2,3-DMB	2,3-DMB	TOLUENE	TOLUENE	M-XYL	M-XYL
SIDE	1	SIDE	1	SIDE	2	SIDE	1	SIDE	2	SIDE	1	SIDE	2	SIDE
0.00	-202.	0.0	0.0	0.0	0.0	0.0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.20	-200.	0.0	0.0	0.0	0.0	0.0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.35	-185.	***	***	***	***	***	***	***	***	***	***	***	***	***
0.42	-148.	***	***	***	***	***	***	***	***	***	***	***	***	***
0.24	-136.	***	***	***	***	***	***	***	***	***	***	***	***	***
0.30	-130.	***	***	***	0.0133	0.0	0.0102	0.0102	0.0102	0.0102	0.0102	0.0102	0.0102	0.0102
0.49	-111.	***	***	***	***	***	***	***	***	***	***	***	***	***
0.51	-109.	***	***	***	***	***	***	***	***	***	***	***	***	***
0.58	-102.	***	***	***	***	***	***	***	***	***	***	***	***	***
0.10	-90.	0.0140	0.0	0.0	0.0103	0.0103	0.0103	0.0103	0.0103	0.0103	0.0103	0.0103	0.0103	0.0103
0.11	-89.	***	***	***	***	***	***	***	***	***	***	***	***	***
0.12	-88.	***	***	***	***	***	***	***	***	***	***	***	***	***
0.15	-85.	***	***	***	***	***	***	***	***	***	***	***	***	***
0.25	-75.	***	***	***	***	***	***	***	***	***	***	***	***	***
0.30	-70.	***	***	***	***	***	***	***	***	***	***	***	***	***
0.45	-55.	***	***	***	***	***	***	***	***	***	***	***	***	***
0.50	-50.	***	***	***	***	***	***	***	***	***	***	***	***	***
0.55	-45.	***	***	***	0.0137	0.0	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100
0.57	-43.	***	***	***	***	***	***	***	***	***	***	***	***	***
0.70	-70.	***	***	***	***	***	***	***	***	***	***	***	***	***
1.16	-24.	***	***	***	***	***	***	***	***	***	***	***	***	***
1.22	-18.	***	***	***	***	***	***	***	***	***	***	***	***	***
1.40	0.	***	***	***	***	***	***	***	***	***	***	***	***	***
1.45	5.	***	***	***	***	***	***	***	***	***	***	***	***	***
1.55	15.	***	***	***	***	***	***	***	***	***	***	***	***	***
1.215	35.	0.0106	***	***	0.0001	0.0001	0.0062	0.0062	0.0062	0.0062	0.0062	0.0062	0.0062	0.0062
1.216	36.	***	***	***	***	***	***	***	***	***	***	***	***	***
1.229	49.	***	***	***	***	***	***	***	***	***	***	***	***	***
1.244	64.	***	***	***	***	***	***	***	***	***	***	***	***	***
1.246	66.	***	***	***	***	***	***	***	***	***	***	***	***	***
1.300	80.	***	***	***	0.0074	0.0	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023
1.315	95.	***	***	***	***	***	***	***	***	***	***	***	***	***
1.330	110.	***	***	***	***	***	***	***	***	***	***	***	***	***
1.345	125.	0.0057	***	***	0.0000	0.0000	0.0014	0.0014	0.0014	0.0014	0.0014	0.0014	0.0014	0.0014
1.356	136.	***	***	***	***	***	***	***	***	***	***	***	***	***
1.415	155.	***	***	***	***	***	***	***	***	***	***	***	***	***
1.426	166.	***	***	***	0.0040	0.0	0.0006	0.0006	0.0006	0.0006	0.0006	0.0006	0.0006	0.0006
1.430	170.	***	***	***	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001
1.432	172.	***	***	***	***	***	***	***	***	***	***	***	***	***
1.445	185.	***	***	***	***	***	***	***	***	***	***	***	***	***
1.529	229.	***	***	***	***	***	***	***	***	***	***	***	***	***
1.545	245.	***	***	***	***	***	***	***	***	***	***	***	***	***
1.600	260.	***	***	***	0.0018	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001
1.615	275.	***	***	***	***	***	***	***	***	***	***	***	***	***
1.631	291.	***	***	***	***	***	***	***	***	***	***	***	***	***
1.644	304.	***	***	***	***	***	***	***	***	***	***	***	***	***
1.645	305.	0.0008	***	***	0.0001	0.0001	0.0002	0.0002	0.0002	0.0002	0.0002	0.0002	0.0002	0.0002
1.650	310.	***	***	***	***	***	***	***	***	***	***	***	***	***

BAG-104  
DIAE SURROGATE RUN #4  
1979 OCT 23

CLKCK TIME	ELAPSED TIME (MIN)	B-SCAT	CONDENS.	CONDENS.	AEROSL N	AEROSL N	AEROSL S	AEROSL S	AEROSL V	AEROSL V	TS DEG F	TS DEG F	UV
018	-202.	0.20	*****	*****	0.03	*****	0.53	*****	0.04	*****	0.06	*****	*****
020	-200.	*****	*****	*****	0.03	*****	*****	*****	0.05	*****	0.06	*****	*****
025	-185.	*****	*****	*****	0.02	*****	0.20	*****	0.05	*****	0.14	*****	*****
035	-136.	*****	*****	*****	0.20	*****	0.55	*****	0.06	*****	0.14	*****	*****
040	-140.	*****	*****	*****	0.20	*****	0.20	*****	0.41	*****	0.05	*****	*****
045	-130.	*****	*****	*****	0.20	*****	0.20	*****	0.05	*****	0.05	*****	*****
050	-111.	0.20	*****	*****	0.20	*****	0.34	*****	0.06	*****	0.14	*****	*****
051	-109.	*****	*****	*****	0.20	*****	0.10	*****	0.27	*****	2.46	*****	*****
058	-102.	*****	*****	*****	0.20	*****	0.20	*****	0.77	*****	0.27	*****	71.3
1010	-90.	*****	*****	*****	0.20	*****	0.20	*****	0.02	*****	0.02	*****	*****
1011	-89.	*****	*****	*****	0.20	*****	0.11	*****	0.07	*****	0.37	*****	*****
1012	-88.	*****	*****	*****	0.20	*****	0.20	*****	0.42	*****	0.02	*****	78.5
1015	-85.	0.20	*****	*****	0.20	*****	0.10	*****	0.42	*****	*****	*****	*****
1025	-75.	*****	*****	*****	0.20	*****	0.20	*****	0.11	*****	1.17	*****	*****
1030	-70.	*****	*****	*****	0.20	*****	0.10	*****	0.76	*****	69.5	*****	*****
1045	-55.	0.20	*****	*****	0.20	*****	0.11	*****	0.07	*****	0.37	*****	*****
1050	-50.	*****	*****	*****	0.20	*****	0.10	*****	0.42	*****	0.02	*****	78.5
1055	-45.	*****	*****	*****	0.20	*****	0.20	*****	0.07	*****	0.37	*****	*****
1057	-43.	*****	*****	*****	0.20	*****	0.10	*****	0.11	*****	1.17	*****	*****
1115	-25.	0.30	*****	*****	0.01	*****	0.60	*****	0.06	*****	0.09	*****	71.3
1116	-24.	*****	*****	*****	0.20	*****	0.10	*****	0.27	*****	0.35	*****	73.1
1122	-18.	*****	*****	*****	0.20	*****	0.20	*****	0.27	*****	0.27	*****	*****
1140	0.	*****	*****	*****	0.20	*****	0.30	*****	0.49	*****	2.71	*****	*****
1145	5.	0.20	*****	*****	0.20	*****	21.00	*****	1.40	*****	0.34	*****	76.7
1155	15.	*****	*****	*****	0.20	*****	0.10	*****	0.35	*****	0.35	*****	0.041
1215	35.	0.50	*****	*****	22.00	*****	56.10	*****	16.00	*****	40.60	*****	76.7
1216	36.	*****	*****	*****	0.50	*****	0.50	*****	0.53	*****	0.53	*****	*****
1229	43.	0.30	*****	*****	0.30	*****	0.20	*****	0.49	*****	0.49	*****	70.5
1244	64.	*****	*****	*****	0.20	*****	0.20	*****	0.35	*****	0.35	*****	*****
1246	66.	0.70	*****	*****	19.00	*****	49.50	*****	22.30	*****	67.90	*****	80.3
1309	80.	*****	*****	*****	0.20	*****	0.10	*****	0.53	*****	0.16	*****	78.5
1315	95.	1.00	*****	*****	17.00	*****	44.10	*****	24.40	*****	82.10	*****	0.034
1330	110.	*****	*****	*****	0.30	*****	0.10	*****	0.61	*****	1.92	*****	0.3
1345	125.	1.30	*****	*****	15.00	*****	40.30	*****	24.70	*****	90.00	*****	0.037
1356	136.	0.30	*****	*****	0.10	*****	0.10	*****	0.46	*****	0.20	*****	80.3
1415	155.	1.20	*****	*****	1.3.00	*****	37.70	*****	21.20	*****	76.50	*****	0.037
1426	160.	0.30	*****	*****	0.30	*****	0.10	*****	1.44	*****	0.70	*****	70.5
1430	170.	0.70	*****	*****	9.00	*****	9.00	*****	0.61	*****	0.61	*****	0.031
1432	172.	0.30	*****	*****	0.30	*****	0.10	*****	24.70	*****	0.34	*****	80.3
1445	185.	1.00	*****	*****	11.00	*****	29.20	*****	17.80	*****	63.90	*****	78.5
1455	195.	0.30	*****	*****	0.10	*****	0.10	*****	0.24	*****	0.26	*****	80.3
1500	200.	0.50	*****	*****	0.00	*****	0.00	*****	1.44	*****	3.55	*****	0.021
1515	215.	0.70	*****	*****	9.00	*****	25.50	*****	13.60	*****	46.20	*****	*****
1527	227.	0.30	*****	*****	0.30	*****	0.10	*****	0.56	*****	0.29	*****	82.1
1529	229.	0.20	*****	*****	0.20	*****	0.20	*****	1.78	*****	0.20	*****	0.028
1545	245.	0.50	*****	*****	0.30	*****	0.10	*****	0.34	*****	0.11	*****	78.5
1590	260.	0.40	*****	*****	7.00	*****	1.00	*****	6.93	*****	19.90	*****	0.025
1615	275.	0.40	*****	*****	0.40	*****	0.90	*****	1.21	*****	1.75	*****	0.022
1631	291.	0.40	*****	*****	6.40	*****	6.70	*****	5.83	*****	14.50	*****	78.5
1644	304.	0.40	*****	*****	6.40	*****	6.70	*****	5.83	*****	14.50	*****	0.012
1645	305.	0.30	*****	*****	0.30	*****	0.10	*****	0.13	*****	0.03	*****	74.9
1659	310.	0.30	*****	*****	0.30	*****	0.10	*****	0.13	*****	0.02	*****	*****

BAG-105  
DMAE SURROGATE RUN #5  
1979 OCT 31

0630-0800 BAG FILLED WITH PURE AIR FROM CHAMBER SYSTEM  
BAG VOLUME APPROXIMATELY 31 CUBIC METERS  
BAG TURNED END FOR END TO VERIFY THAT ENHANCED RATE  
NOT DUE TO DIFFERENCES FROM SIDE TO SIDE (LIGHT INTENSITY, ETC.)  
BAG COVERED  
RH IS 14% AT 21 DEG C  
0900 2.6 ML NO2 INJECTED AND MIXED  
0901 7.3 ML NO2 INJECTED AND MIXED  
0903 500 ML SURROGATE J INJECTED AND MIXED  
0906 14.0 MICROLITERS (U-L) 2.3CMB, 1.9 U-L TOLUENE,  
1.6 U-L 2ME-2-C4, 5.4 U-L M-XYLENE INJECTED AND MIXED  
0910 BAG DIVIDED  
0915 7.2 U-L DMAE INJECTED INTO SIDE 2  
0940 (0.11 PPM, CALCULATED)  
1015 BAG UNCOVERED

\*MEASUREMENTS SO MARKED INCLUDE THE FOLLOWING UNITS AND FACTORS:  
B-SCAT (METERS-1) X E+4  
CONDENSATION NUCLEI (PART/CUBIC CM) X E-3  
AEROSOL NUMBER (PART/CUBIC CM) X E-3  
AEROSOL SURFACE (U-METERS2/CUBIC CM) X E-2  
AEROSOL VOLUME (CUBIC U-METERS/CUBIC CM) X 1  
UV (CAL/CM2-MIN) X 1

T=0 AT 1015 PST

TS DEG K AVERAGE 299.0  
UV AVERAGE 0.004

\* ASSIGNED INITIAL CONDITION

BAG-105  
DMAE SURROGATE RUN #5  
1979 OCT 31

CLICK	ELAPSED	OZONE	OZONE	OZONE	OZONE	OZONE	OZONE	OZONE	OZONE	NO	NO2-CORR	NO2-CORR	NOx-CORR	NOx-CORR
TIME	Y(MIN)	PPM	PPM	PPM	PPM	PPM	PPM	PPM	PPM	SIDE 1	SIDE 2	SIDE 1	SIDE 2	SIDE 1
		DAS-1	DAS-2	BNX-1	BNX-2	SIDE 1	SIDE 2	SIDE 1	SIDE 2	0.0	0.0	0.0	0.0	0.0
850.	-85.	***	0.010	***	0.0	***	0.0	***	0.0	0.083	0.083	0.231	0.231	0.231
920.	-55.	***	0.008	***	0.001	***	0.150	***	0.150	0.086	0.086	0.229	0.229	0.229
950.	-25.	***	0.008	***	0.001	***	0.150	***	0.150	0.086	0.086	0.232	0.232	0.232
955.	-20.	0.0	***	0.0	***	0.153	***	0.153	0.086	0.086	0.232	0.232	0.232	0.232
1000.	-15.	***	***	***	***	***	***	***	***	***	***	***	***	***
1009.	-6.	***	***	***	***	***	***	***	***	***	***	***	***	***
1030.	15.	0.010	***	0.009	0.009	0.142	***	0.142	***	0.093	0.093	0.230	0.230	0.230
1039.	24.	***	0.010	***	0.011	***	0.129	***	0.129	0.099	0.099	0.221	0.221	0.221
1050.	35.	***	***	***	***	***	***	***	***	***	***	***	***	***
1100.	45.	0.013	***	0.013	0.013	0.112	***	0.112	***	0.110	0.110	0.227	0.227	0.227
1109.	54.	***	***	***	***	0.014	***	0.014	***	0.100	0.100	0.216	0.216	0.216
1111.	56.	***	***	***	***	0.017	***	0.017	***	0.093	0.093	0.210	0.210	0.210
1115.	60.	***	***	***	***	0.021	***	0.021	***	0.093	0.093	0.209	0.209	0.209
1130.	75.	0.022	***	0.021	0.021	0.091	***	0.091	***	0.139	0.139	0.212	0.212	0.212
1131.	76.	***	***	***	***	0.024	***	0.024	***	0.139	0.139	0.212	0.212	0.212
1139.	84.	***	***	***	***	0.030	***	0.030	***	0.071	0.071	0.201	0.201	0.201
1146.	91.	***	***	***	***	0.033	***	0.033	***	0.059	0.059	0.195	0.195	0.195
1200.	135.	0.031	***	0.031	0.031	0.037	***	0.037	***	0.049	0.049	0.155	0.155	0.155
1209.	114.	***	0.044	***	0.044	***	0.058	***	0.058	***	0.058	0.196	0.196	0.196
1215.	120.	***	***	***	***	0.055	***	0.055	***	0.058	0.058	0.160	0.160	0.160
1230.	135.	0.045	***	0.045	0.044	0.040	***	0.040	***	0.166	0.166	0.198	0.198	0.198
1238.	143.	0.056	***	0.053	0.053	0.029	***	0.029	***	0.156	0.156	0.208	0.208	0.208
1245.	150.	***	***	***	***	0.059	***	0.059	***	0.157	0.157	0.212	0.212	0.212
1300.	162.	0.056	***	0.058	0.058	0.029	***	0.029	***	0.155	0.155	0.212	0.212	0.212
1307.	172.	***	***	0.079	0.079	0.071	***	0.071	***	0.139	0.139	0.201	0.201	0.201
1315.	180.	***	***	***	***	0.054	***	0.054	***	0.071	0.071	0.201	0.201	0.201
1330.	195.	0.067	***	0.071	0.071	0.020	***	0.020	***	0.175	0.175	0.208	0.208	0.208
1340.	205.	***	0.097	***	0.089	0.089	0.011	***	0.011	***	0.153	0.153	0.153	0.153
1345.	210.	***	***	***	***	0.011	***	0.011	***	0.173	0.173	0.173	0.173	0.173
1400.	225.	0.076	***	0.082	0.082	0.015	***	0.015	***	0.171	0.171	0.177	0.177	0.177
1409.	234.	***	0.110	***	0.104	0.010	***	0.010	***	0.175	0.175	0.186	0.186	0.186
1415.	240.	***	***	***	***	0.089	***	0.089	***	0.011	0.011	0.153	0.153	0.153
1430.	255.	0.083	***	0.089	0.089	0.011	***	0.011	***	0.171	0.171	0.173	0.173	0.173
1435.	264.	***	0.117	***	0.120	0.012	***	0.012	***	0.002	0.002	0.137	0.137	0.137
1454.	279.	***	***	***	***	0.100	***	0.100	***	0.008	0.008	0.175	0.175	0.175
1500.	285.	0.090	***	0.100	0.100	0.008	***	0.008	***	0.002	0.002	0.132	0.132	0.132
1508.	293.	***	0.120	***	0.126	0.002	***	0.002	***	0.132	0.132	0.130	0.130	0.130

BAG-105  
DMAE SURROGATE PUN #5  
1979 OCT 31

CLK/CLOCK	ELAPSED TIME	DMAE PPM	ACETONE PPM	MEK PPM	NEK PPM	METHANE		ETHANE		ETHENE	
						SIDE 1	SIDE 2	SIDE 1	SIDE 2	SIDE 1	SIDE 2
850	-85.	* *** ****	* *** ****	0.0044	0.0044	*****	*****	*****	*****	****	****
920	-55.	* *** ****	* *** ****	0.0044	0.0044	*****	*****	1.40	1.40	0.0448	0.0448
950	-25.	* *** ****	* *** ****	0.0044	0.0044	*****	*****	*****	*****	****	****
955	-20.	* *** ****	* *** ****	0.0044	0.0044	*****	*****	*****	*****	****	****
1000	-15.	6.500C	* *** ****	0.0044	0.0044	*****	*****	*****	*****	****	****
1009	-6.	4.6000	* *** ****	0.0044	0.0044	*****	*****	*****	*****	****	****
1230	15.	3.3000	0.0076	0.0044	0.0044	*****	*****	1.38	1.38	0.0433	0.0433
1039	24.	* *** ****	* *** ****	0.0044	0.0044	*****	*****	*****	*****	****	****
1050	35.	C.0	* *** ****	0.0044	0.0044	*****	*****	*****	*****	****	****
1100	45.	* *** ****	* *** ****	0.0044	0.0044	*****	*****	*****	*****	****	****
1109	54.	* *** ****	* *** ****	0.0044	0.0044	*****	*****	*****	*****	****	****
1111	56.	0.0	* *** ****	0.0044	0.0044	*****	*****	*****	*****	****	****
1115	60.	* *** ****	* *** ****	0.0099	0.0099	*****	*****	0.0016	0.0016	1.40	1.40
1130	75.	* *** ****	* *** ****	0.0044	0.0044	*****	*****	*****	*****	****	****
1131	76.	0.0	* *** ****	0.0044	0.0044	*****	*****	*****	*****	****	****
1139	84.	* *** ****	* *** ****	0.0044	0.0044	*****	*****	*****	*****	****	****
1146	91.	0.0	* *** ****	0.0044	0.0044	*****	*****	*****	*****	****	****
1200	105.	* *** ****	0.0171	0.0028	0.0028	*****	*****	0.0016	0.0016	0.0718	0.0718
1209	114.	* *** ****	* *** ****	0.0044	0.0044	*****	*****	*****	*****	****	****
1215	120.	0.0	* *** ****	0.0044	0.0044	*****	*****	*****	*****	****	****
1230	135.	* *** ****	* *** ****	0.0044	0.0044	*****	*****	*****	*****	****	****
1236	143.	* *** ****	* *** ****	0.0044	0.0044	*****	*****	*****	*****	****	****
1245	150.	0.0	* *** ****	0.0169	0.0169	*****	*****	0.0026	0.0026	0.0730	0.0730
1300	165.	* *** ****	* *** ****	0.0044	0.0044	*****	*****	*****	*****	****	****
1307	172.	* *** ****	* *** ****	0.0044	0.0044	*****	*****	*****	*****	****	****
1315	180.	0.0	* *** ****	0.0044	0.0044	*****	*****	*****	*****	****	****
1330	195.	* *** ****	0.0219	0.0044	0.0044	*****	*****	1.34	1.34	0.0334	0.0334
1340	205.	* *** ****	* *** ****	0.0044	0.0044	*****	*****	*****	*****	****	****
1345	210.	* *** ****	* *** ****	0.0044	0.0044	*****	*****	*****	*****	****	****
1400	225.	* *** ****	* *** ****	0.0044	0.0044	*****	*****	*****	*****	****	****
1409	234.	* *** ****	* *** ****	0.0044	0.0044	*****	*****	*****	*****	****	****
1415	240.	* *** ****	* *** ****	0.0195	0.0195	*****	*****	0.0040	0.0040	1.30	1.30
1430	255.	* *** ****	* *** ****	0.0044	0.0044	*****	*****	*****	*****	****	****
1439	264.	* *** ****	* *** ****	0.0044	0.0044	*****	*****	*****	*****	****	****
1454	279.	* *** ****	* *** ****	0.0044	0.0044	*****	*****	*****	*****	****	****
1500	285.	* *** ****	* *** ****	0.0044	0.0044	*****	*****	*****	*****	****	****
1508	293.	* *** ****	* *** ****	0.0044	0.0044	*****	*****	*****	*****	****	****

BAG-105  
DNAE SURROGATE RUN #5  
1979 OCT 31

TIME	ELAPSED TIME	ACETYLEN	ACETYLEN	ACETYLEN	PROPANE	PROPENE	PROPENYL	PROPENYL	1-C4	1-C4
050	-85.	(PN-1)	(PN-2)	(DMS-1)	SIDE 1	SIDE 2	SIDE 1	SIDE 2	SIDE 1	SIDE 2
920	-55.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
950	-25.	* * * * *	* * * * *	* * * * *	0.0482	0.0317	0.0113	0.0012	0.171	0.0001
955	-20.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1000	-15.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1009	-6.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1030	15.	0.0459	* * * * *	0.0195	0.0322	0.011	* * * * *	* * * * *	* * * * *	* * * * *
1039	24.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1050	35.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1100	45.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1109	54.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1111	56.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1115	60.	* * * * *	0.0471	* * * * *	0.0473	0.0312	* * * * *	0.010	* * * * *	0.165
1130	75.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1131	76.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1139	84.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1146	91.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1200	105.	0.0483	* * * * *	0.0477	* * * * *	0.0317	* * * * *	0.008	* * * * *	0.0002
1209	114.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1215	120.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1230	135.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1233	143.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1245	150.	* * * * *	0.0466	* * * * *	0.0469	0.0309	* * * * *	0.008	* * * * *	0.162
1300	165.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1307	172.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1315	180.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1330	195.	0.0475	* * * * *	0.0473	* * * * *	0.0310	* * * * *	0.005	* * * * *	0.0001
1340	205.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1345	210.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1400	225.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1409	234.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1415	240.	* * * * *	0.0463	* * * * *	0.0456	0.0299	* * * * *	0.005	* * * * *	0.0001
1430	252.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1439	264.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1454	279.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1500	285.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1508	293.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *

BAG-105  
D-ME SUPROGATE RUN #5  
1979 OCT 31

CLKICK	ELAPSED TIME (MIN)	I-C4=	T2-C4=	I-C5	CIS2-C4=	CIS2-C4=	N-C5	2MF-C4=2	2MF-C4=2
SIDE 1	SIDE 2	SIDE 1	SIDE 2	SIDE 1	SIDE 2	SIDE 1	SIDE 2	SIDE 1	SIDE 2
PPM	PPM	PPM	PPM	PPM	PPM	PPM	PPM	PPM	PPM
850	-85.	***	***	***	***	***	***	***	***
920	-55.	0.0001	0.0001	0.0006	0.0006	0.0003	0.0005	0.0129	0.0002
950	-25.	***	***	***	***	***	***	0.0002	0.00220
955	-20.	***	***	***	***	***	***	***	***
1000	-15.	***	***	***	***	***	***	***	***
1009	-6.	***	***	***	***	***	***	***	***
1030	15.	0.0001	0.0005	0.0002	0.0002	0.0002	0.0002	0.0116	0.0002
1039	24.	***	***	***	***	***	***	***	***
1050	35.	***	***	***	***	***	***	***	***
1100	45.	***	***	***	***	***	***	***	***
1109	54.	***	***	***	***	***	***	***	***
1111	56.	***	***	***	***	***	***	***	***
1115	60.	***	***	0.0001	0.0004	0.0008	0.0008	0.0087	0.0003
1130	75.	***	***	***	***	***	***	***	***
1131	76.	***	***	***	***	***	***	***	***
1139	84.	***	***	***	***	***	***	***	***
1146	91.	***	***	***	***	***	***	***	***
1200	105.	0.0001	0.0002	0.0002	0.0002	0.0008	0.0008	0.0001	0.0007
1209	114.	***	***	***	***	***	***	***	***
1215	120.	***	***	***	***	***	***	***	***
1230	135.	***	***	***	***	***	***	***	***
1238	143.	***	***	***	***	***	***	***	***
1245	150.	***	***	***	***	***	***	***	***
1300	165.	***	***	***	***	***	***	***	***
1307	172.	***	***	***	***	***	***	***	***
1315	180.	***	***	***	***	***	***	***	***
1330	195.	0.0000	0.0001	0.0001	0.0002	0.0006	0.0006	0.0030	0.0004
1340	205.	***	***	***	***	***	***	***	***
1345	210.	***	***	***	***	***	***	***	***
1400	225.	***	***	***	***	***	***	***	***
1409	234.	***	***	***	***	***	***	***	***
1415	240.	***	***	0.0001	0.0001	0.0002	0.0002	0.0003	0.0001
1430	255.	***	***	***	***	***	***	***	***
1439	264.	***	***	***	***	***	***	***	***
1454	279.	***	***	***	***	***	***	***	***
1500	285.	***	***	***	***	***	***	***	***
1508	293.	***	***	***	***	***	***	***	***

BAG-105  
DIAE SURROGATE RUN #5  
1979 OCT 31

CLOCK	ELAPSED	2,3-DMD	2,3-DMU	TOLUENE	TOLUENE	N-XYL
TIME	T(MIN)	PPM	PPM	PPM	PPM	PPM
		SIDE 1	SIDE 2	SIDE 1	SIDE 2	SIDE 1
050	-85.	*****	*****	*****	*****	*****
020	-55.	0.0761	0.0761	0.014	0.014	0.0329
950	-25.	*****	*****	*****	*****	*****
955	-20.	*****	*****	*****	*****	*****
1000	-15.	*****	*****	*****	*****	*****
1009	-6.	*****	*****	*****	*****	*****
1030	15.	0.0774	*****	0.014	*****	*****
1039	24.	*****	*****	*****	*****	*****
1050	35.	*****	*****	*****	*****	*****
1100	45.	*****	*****	*****	*****	*****
1109	54.	*****	*****	*****	*****	*****
1111	56.	*****	*****	*****	*****	*****
1115	60.	*****	0.0731	*****	0.013	*****
1130	75.	*****	*****	*****	*****	*****
1131	76.	*****	*****	*****	*****	*****
1139	84.	*****	*****	*****	*****	*****
1146	91.	*****	*****	*****	*****	*****
1200	105.	0.0710	*****	0.012	*****	0.0304
1209	114.	*****	*****	*****	*****	*****
1215	120.	*****	*****	*****	*****	*****
1230	135.	*****	*****	*****	*****	*****
1238	143.	*****	*****	*****	*****	*****
1245	150.	*****	0.0692	*****	0.012	0.0244
1300	165.	*****	*****	*****	*****	*****
1307	172.	*****	*****	*****	*****	*****
1315	180.	*****	*****	*****	*****	*****
1330	195.	0.0666	*****	0.011	*****	0.0190
1340	205.	*****	*****	*****	*****	*****
1345	210.	*****	*****	*****	*****	*****
1400	225.	*****	*****	*****	*****	*****
1409	234.	*****	*****	*****	*****	*****
1415	240.	*****	0.0651	*****	0.011	0.0192
1430	255.	*****	*****	*****	*****	*****
1439	264.	*****	*****	*****	*****	*****
1454	279.	*****	*****	*****	*****	*****
1500	285.	*****	*****	*****	*****	*****
1508	293.	*****	*****	*****	*****	*****

BAG-105  
DMAE SURROGATE RUN #5  
1979 OCT 31

CLOCK TIME	ELAPSED TIME (MIN)	B-SCAT	CONDENS.	CONDENS.	AEROSL N	AEROSL S	AEROSL V	TS	DEG F	DEG F	UV
050	-85.	0.40	*****	*****	1.30	*****	1.73	*****	0.69	*****	*
920	-55.	0.40	*****	*****	1.10	*****	1.77	*****	0.53	*****	69.5
950	-25.	0.40	*****	*****	1.60	*****	3.10	*****	0.74	*****	2.58
955	-20.	0.30	*****	*****	0.80	*****	1.72	*****	0.26	*****	2.93
1000	-15.	*****	*****	*****	*****	*****	*****	*****	0.77	*****	*****
1009	-6.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1030	15.	0.30	*****	*****	0.20	*****	1.67	*****	0.33	*****	1.59
1039	24.	0.40	*****	*****	43.00	*****	119.00	*****	10.90	*****	39.90
1050	35.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1100	45.	0.40	*****	*****	1.30	*****	2.00	*****	0.38	*****	1.26
1109	54.	*****	*****	0.70	*****	40.00	*****	99.50	*****	31.30	*****
1111	56.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1115	60.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1130	75.	0.30	*****	*****	0.20	*****	1.47	*****	0.46	*****	2.04
1131	76.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1139	84.	*****	*****	1.40	*****	36.00	*****	70.20	*****	48.10	*****
1146	91.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1200	105.	0.30	*****	*****	0.10	*****	1.09	*****	0.17	*****	0.55
1209	114.	*****	*****	2.50	*****	30.00	*****	82.60	*****	51.30	*****
1215	120.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1230	135.	0.30	*****	*****	0.20	*****	1.37	*****	0.25	*****	0.75
1238	143.	*****	*****	4.30	*****	26.00	*****	71.30	*****	58.40	*****
1245	150.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1300	165.	0.30	*****	*****	0.30	*****	1.14	*****	0.22	*****	0.53
1307	172.	*****	*****	5.90	*****	24.00	*****	64.00	*****	60.70	*****
1315	180.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1330	195.	0.30	*****	*****	0.10	*****	0.98	*****	0.32	*****	1.67
1340	205.	*****	*****	6.50	*****	21.00	*****	53.40	*****	56.30	*****
1345	210.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1400	225.	0.30	*****	*****	0.30	*****	1.06	*****	0.23	*****	0.75
1409	234.	*****	*****	6.00	*****	19.00	*****	48.70	*****	49.50	*****
1415	240.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1430	255.	0.30	*****	*****	0.20	*****	0.77	*****	0.50	*****	3.79
1439	264.	*****	*****	4.90	*****	16.00	*****	40.00	*****	42.10	*****
1454	279.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1500	285.	0.30	*****	*****	0.40	*****	1.14	*****	0.28	*****	1.48
1508	293.	*****	*****	3.80	*****	13.00	*****	35.70	*****	33.60	*****

BAG-201  
SURROGATE CONTRACT #1  
1979 OCT 24

TIME (PDT)  
0930-1100 BAG #11 FILLED WITH PURE AIR FROM CHAMBER SYSTEM. DRY  
0940 BAG COVERED  
1119 2.6 ML NO.2 INJECTED AND MIXED  
1132 5.00 ML SURROGATE J INJECTED  
1137 1.6 MICROLITERS (U-L) 2MEC4 = 1.9 U-L TOLUENE, 5.4 U-L M-XYLENE  
1144 KH LESS THAN 10% PURE AIR ON DRY BY MISTAKE!  
1150 BAG MIXED THOROUGHLY AND DIVIDED  
1221 BAG UNCOVERED  
1332 DUE TO LEAK IN SIDE 2, BAG WAS UNDIVIDED, ADJUSTED FOR EQUAL  
VOLUMES AND REDIVIDED (SIDE 1 ALMOST EMPTY AT TIME)

\*MEASUREMENTS SO MARKED INCLUDE THE FOLLOWING UNITS AND FACTORS:  
B-SCAT (METERS-1) X E+4  
CONDENSATION NUCLEI (PART/CUBIC CM) X E-3  
AEROSOL NUMBER (PART/CUBIC CM) X E-3  
AEROSOL SURFACE (U-METERS2/CUBIC CM) X E-2  
AEROSOL VOLUME (CUBIC U-METERS/CUBIC CM) X 1  
UV (CAL/CM2-MIN) X 1

T=0 AT 1220 PST

VS DEG K AVERAGE 300.4  
UV AVERAGE 0.004

\* ASSIGNED INITIAL CONDITION

BAG-201  
SURROGATE CONTROL #1  
1979 OCT 24

CLOCK TIME	FLAPS/TIME	OZONE	OZONE	NO	NO2-CORR	NO2-CORR	NOX-CORR	NOX-CORR	PPM	
									PPM	PPM
11:09	-71.	0.0	DAS-1	DAS-2	BNX-1	BNX-2	SIDE 1	SIDE 2	0.0	0.0
11:10	-70.	***	***	***	***	***	***	***	***	***
11:50	-30.	***	***	***	***	***	***	***	***	***
12:00	-20.	***	***	0.001	***	0.001	***	0.168	***	0.280
12:08	-12.	0.004	***	0.001	***	0.001	***	0.115	***	0.281
12:30	10.	0.007	***	0.010	***	0.010	***	0.117	***	0.277
12:39	13.	0.009	***	0.008	***	0.008	***	0.155	***	0.275
13:00	40.	0.012	***	0.014	***	0.014	***	0.148	***	0.269
13:10	50.	***	***	0.010	***	0.010	***	0.124	***	0.266
13:15	55.	***	***	***	***	***	***	***	***	***
13:30	70.	0.018	***	0.020	***	0.020	***	0.173	***	0.259
13:37	77.	***	***	0.016	***	0.020	***	0.178	***	0.255
14:00	100.	0.027	***	0.031	***	0.031	***	0.196	***	0.249
14:14	114.	***	***	0.025	***	0.027	***	0.050	***	0.243
14:30	130.	0.040	***	0.040	***	0.040	***	0.203	***	0.238
14:42	142.	***	***	0.031	***	0.033	***	0.040	***	0.239
14:45	145.	***	***	***	***	***	***	***	***	***
15:00	160.	0.043	***	0.051	***	0.051	***	0.208	***	0.231
15:14	174.	***	***	0.035	***	0.038	***	0.029	***	0.237
15:30	190.	0.052	***	0.057	***	0.057	***	0.217	***	0.229
15:44	204.	***	***	0.037	***	0.041	***	0.020	***	0.217
16:00	220.	0.052	***	0.060	***	0.060	***	0.217	***	0.221
16:13	233.	***	***	0.037	***	0.042	***	0.011	***	0.224
16:15	235.	***	***	***	***	***	***	***	***	***
16:32	252.	0.052	***	0.059	***	0.059	***	0.005	***	0.217
16:45	265.	***	***	0.038	***	0.040	***	0.007	***	0.220
17:00	280.	***	***	***	***	***	***	***	***	***

BAG-201  
SURROGATE CONTROL #1  
1973 OCT 24

CLOCK	ELAPSED TIME T(MIN)	PAN PPM	PAN PPM	ACETONE PPM	ACETONE PPM	MEK PPM	MEK PPM	METHANE PPM	METHANE PPM	ETHANE PPM	ETHANE PPM
	SIDE 1	SIDE 2	SIDE 1	SIDE 2	SIDE 1	SIDE 2	SIDE 1	SIDE 2	SIDE 1	SIDE 2	SIDE 1
11.09	-71.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
11.10	-70.	*****	*****	0.0015	0.0015	*****	*****	1.56	1.56	0.0079	0.0079
11.50	-30.	*****	*****	0.0067	0.0067	0.0004	0.0004	1.55	1.55	0.0478	0.0478
12.00	-20.	*****	0.0	*****	*****	*****	*****	*****	*****	*****	*****
12.08	-12.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
12.30	1.0.	*****	*****	0.0087	0.0087	0.0007	0.0007	1.55	1.55	0.0772	0.0772
12.39	1.9.	0.0	*****	*****	*****	*****	*****	*****	*****	*****	*****
13.00	4.0.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
13.10	5.0.	*****	0.001	*****	*****	0.0013	*****	*****	*****	*****	*****
13.15	5.5.	*****	*****	*****	*****	0.0120	*****	*****	*****	*****	*****
13.30	7.0.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
13.37	7.7.	0.001	*****	*****	*****	*****	*****	*****	*****	*****	*****
14.00	10.0.	*****	0.0191	*****	0.0027	*****	1.54	*****	0.0777	*****	0.0430
14.14	11.4.	*****	0.002	*****	*****	*****	*****	*****	*****	*****	*****
14.30	13.0.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
14.42	14.2.	*****	0.002	*****	*****	*****	*****	*****	*****	*****	*****
14.45	14.5.	*****	*****	0.0192	*****	0.0030	*****	1.55	*****	0.0772	*****
15.00	16.0.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
15.14	17.4.	*****	0.003	*****	*****	*****	*****	*****	*****	*****	*****
15.30	19.0.	*****	0.0253	*****	0.0042	*****	1.55	*****	0.0771	*****	0.0390
15.44	20.4.	*****	0.004	*****	*****	*****	*****	*****	*****	*****	*****
16.00	22.0.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
16.13	23.3.	0.004	*****	*****	*****	*****	*****	*****	*****	*****	0.0395
16.15	23.5.	*****	*****	0.0221	*****	0.0039	*****	1.56	*****	0.0776	*****
16.32	25.2.	0.0	*****	*****	*****	*****	*****	*****	*****	*****	*****
16.45	26.5.	*****	0.004	*****	*****	*****	*****	*****	*****	*****	*****
17.00	29.0.	*****	*****	0.0049	*****	*****	*****	1.56	*****	0.0773	0.0370

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CLOCK	ELAPSED	ACETYLEN	ACETYLEN	ACETYLEN	ACETYLEN	ACETYLEN	PROPANE	PROPANE	PROPANE	PROPANE	PROPANE	PROPENE	PROPENE	I-C4	I-C4	N-C4
							DMS-1	DMS-2	SIDE 1	SIDE 2	SIDE 1	SIDE 2	SIDE 1	SIDE 2	SIDE 1	SIDE 2
11.09	-71.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
11.10	-70.	0.0038	0.0036	0.0036	0.0036	0.0036	0.0247	0.0247	0.001	0.001	0.0013	0.0013	0.0013	0.0013	0.0013	0.0013
11.50	-30.	0.0417	0.0417	0.0400	0.0400	0.0400	0.0358	0.0358	0.012	0.012	0.0014	0.0014	0.0014	0.0014	0.0014	0.0014
12.00	-20.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
12.08	-12.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
12.30	1.0.	0.0455	0.0455	0.0409	0.0409	0.0409	0.0359	0.0359	0.011	0.011	0.0013	0.0013	0.0013	0.0013	0.0013	0.0013
12.39	1.9.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
13.00	4.0.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
13.10	5.0.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
13.15	5.5.	*****	*****	*****	*****	*****	0.0417	0.0404	*****	*****	0.010	0.010	0.010	0.010	0.010	0.010
13.30	7.0.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
13.37	7.7.	*****	*****	*****	*****	*****	0.0398	0.0398	0.0349	0.0349	0.008	0.008	0.008	0.008	0.008	0.008
14.00	100.	0.0409	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
14.14	11.4.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
14.30	13.0.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
14.42	14.2.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
14.45	14.5.	*****	*****	*****	*****	*****	0.0414	0.0396	0.0396	0.0335	0.007	0.007	0.007	0.007	0.007	0.007
15.00	16.0.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
16.14	17.4.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
15.30	19.0.	0.0402	*****	*****	*****	*****	0.0396	0.0396	0.0342	0.0342	0.006	0.006	0.006	0.006	0.006	0.006
15.44	20.4.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
16.00	22.0.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
16.13	23.3.	*****	*****	*****	*****	*****	*****	*****	*****	*****	0.0344	0.0344	0.006	0.006	0.006	0.006
16.15	23.5.	*****	*****	*****	*****	*****	0.0415	0.0387	0.0387	0.0344	0.014	0.014	0.014	0.014	0.014	0.014
16.32	25.2.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
16.45	26.5.	*****	*****	*****	*****	*****	0.0410	0.0387	0.0387	0.0342	0.005	0.005	0.005	0.005	0.005	0.005
17.00	28.0.	*****	*****	*****	*****	*****	0.0410	0.0387	0.0387	0.0342	0.014	0.014	0.014	0.014	0.014	0.014

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SURROGATE CONTROL #1  
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CLOCK TIME	ELAPSED TIME (MIN)	1-C4=		I-C4=		T2-C4=		1-C5		T2-C4=		CIS2-C4=		N-C5	
		PPM	SIDE 1	PPM	SIDE 2	PPM	SIDE 1	PPM	SIDE 2	PPM	SIDE 1	PPM	SIDE 2	PPM	SIDE 1
1109	-71.	* * * * *	0.0002	0.0002	0.0001	0.0001	0.0	0.0002	0.0	0.0	0.0	0.0	0.0	0.0001	0.0001
1110	-70.	0.0001	0.0001	0.0001	0.0001	0.0	0.0	0.0002	0.0	0.0	0.0	0.0	0.0	0.0001	0.0001
1150	-30.	0.0001	0.0001	0.0001	0.0001	0.0	0.0	0.0002	0.0	0.0134	0.0134	0.0001	0.0001	0.0001	0.0001
1200	-20.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1200	-12.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1230	1.0.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	0.0011	* * * * *	0.0002	0.0122	* * * * *	* * * * *	* * * * *	* * * * *
1239	1.9.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1300	4.0.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1310	5.0.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1315	5.5.	* * * * *	C.0002	* * * * *	* * * * *	* * * * *	* * * * *	0.0001	* * * * *	* * * * *	0.0001	* * * * *	* * * * *	* * * * *	0.0
1330	7.0.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1337	7.7.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1400	100.	0.0003	0.0002	0.0002	0.0002	0.0002	0.0002	0.0001	0.0002	0.0084	0.0084	0.0002	0.0002	0.0002	0.0002
1414	114.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1430	130.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1442	142.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1445	145.	* * * * *	C.0001	* * * * *	* * * * *	* * * * *	* * * * *	0.0002	* * * * *	* * * * *	0.0025	* * * * *	* * * * *	* * * * *	0.0
1500	160.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1514	174.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1530	190.	0.0001	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	0.0001	* * * * *	0.0010	0.0010	* * * * *	* * * * *	* * * * *	0.0001
1544	204.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1600	220.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1613	233.	* * * * *	C.0001	* * * * *	* * * * *	* * * * *	* * * * *	0.0000	* * * * *	0.0002	0.0010	* * * * *	* * * * *	* * * * *	0.0001
1615	235.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1.32	252.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1645	265.	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	0.0	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *	* * * * *
1700	280.	0.0001	* * * * *	0.0001	* * * * *	0.0	* * * * *	0.0002	* * * * *	0.0002	* * * * *	* * * * *	* * * * *	* * * * *	0.0002

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SURROGATE CONTROL #1  
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CLOCK	ELAPSED	2-ME-C4=2	2-ME-C4=2	2,3-DNB	2,3-DMS	TOLUENE	TOLUENE	M-XYL
TIME	MIN	PPM	PPM	PPM	PPM	PPM	PPM	PPM
		SIDE 1	SIDE 2	SIDE 1	SIDE 2	SIDE 1	SIDE 2	SIDE 1
11.09	-71.	*****	*****	*****	*****	*****	*****	*****
11.10	-70.	0.0	0.0	0.0	0.0	0.0	0.0	0.0
11.50	-30.	0.0112	0.0112	0.0017	0.0017	0.014	0.014	0.0355
12.00	-20.	*****	*****	*****	*****	*****	*****	*****
12.08	-12.	*****	*****	*****	*****	*****	*****	*****
12.30	1.0.	0.0092	*****	0.0007	*****	0.014	*****	0.0344
12.39	1.9.	*****	*****	*****	*****	*****	*****	*****
13.00	4.0.	*****	*****	*****	*****	*****	*****	*****
13.10	5.0.	*****	*****	*****	*****	*****	*****	*****
13.15	5.5.	*****	*****	0.0046	*****	0.0700	*****	0.0306
13.30	7.0.	*****	*****	*****	*****	*****	*****	*****
13.37	7.7.	*****	*****	*****	*****	*****	*****	*****
14.00	100.	0.0009	*****	0.0741	*****	0.013	0.0252	*****
14.14	114.	*****	*****	*****	*****	*****	*****	*****
14.30	130.	*****	*****	*****	*****	*****	*****	*****
14.42	142.	*****	*****	*****	*****	*****	*****	*****
14.45	145.	*****	0.0007	*****	0.0720	*****	0.012	*****
15.00	160.	*****	*****	*****	*****	*****	*****	*****
15.14	174.	*****	*****	*****	*****	*****	*****	*****
15.30	190.	0.0	*****	0.0704	*****	0.012	*****	0.0205
15.44	204.	*****	*****	*****	*****	*****	*****	*****
16.00	220.	*****	*****	*****	*****	*****	*****	*****
16.13	233.	*****	*****	*****	*****	*****	*****	*****
16.15	235.	*****	*****	*****	0.0702	*****	0.012	0.0212
16.32	252.	*****	*****	*****	*****	*****	*****	*****
16.45	265.	*****	*****	*****	*****	*****	*****	*****
17.00	280.	0.0	*****	0.0689	*****	0.012	*****	0.0193

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SURROGATE CONTROL #1  
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TIME T (MIN)	CLOCK ELAPSED	B-SCAT	CONDENS.	CONDENS.	AEROSL N	AEROSL S	AEROSL V	TS	DEG F	DEG F	UV	TS	SIDE 1*	SIDE 2*										
													SIDE 1*	SIDE 2*										
11.09	-71.	0.30	*****	*****	0.30	*****	0.35	*****	0.09	0.22	*****	0.57	*****	*****	*****	0.57	*****	*****	*****	*****	*****	*****	*****	*****
11.10	-70.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
11.50	-30.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
12.00	-20.	*****	*****	*****	0.40	*****	0.10	*****	0.37	*****	0.14	*****	0.87	*****	0.87	*****	0.87	*****	0.87	*****	0.87	*****	0.87	*****
12.08	-12.	0.40	*****	*****	0.10	*****	0.19	*****	0.09	*****	0.04	*****	0.00	*****	0.00	*****	0.00	*****	0.00	*****	0.00	*****	0.00	*****
12.30	1.0.	0.30	*****	*****	0.20	*****	0.44	*****	0.04	*****	0.10	*****	0.10	*****	0.10	*****	0.10	*****	0.10	*****	0.10	*****	0.10	*****
12.39	1.9.	0.40	*****	*****	0.40	*****	0.10	*****	0.27	*****	0.08	*****	0.33	*****	0.33	*****	0.33	*****	0.33	*****	0.33	*****	0.33	*****
13.00	40.	0.40	****	****	0.50	****	0.09	****	0.05	****	0.27	****	0.5	****	0.5	****	0.5	****	0.5	****	0.5	****	0.5	****
13.10	50.	0.30	****	****	0.30	****	0.20	****	0.11	****	0.28	****	1.27	****	1.27	****	1.27	****	1.27	****	1.27	****	1.27	****
13.15	55.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
13.30	70.	0.30	*****	*****	0.30	*****	0.16	*****	0.26	*****	0.08	*****	0.21	*****	0.21	*****	0.21	*****	0.21	*****	0.21	*****	0.21	*****
13.37	77.	0.40	*****	*****	0.40	*****	0.00	*****	0.25	*****	0.05	*****	5.07	*****	5.07	*****	5.07	*****	5.07	*****	5.07	*****	5.07	*****
14.00	100.	0.40	*****	*****	1.00	*****	0.00	*****	0.09	*****	0.01	*****	0.21	*****	0.21	*****	0.21	*****	0.21	*****	0.21	*****	0.21	*****
14.14	114.	0.40	*****	*****	0.40	*****	0.10	*****	0.19	*****	0.11	*****	0.81	*****	0.81	*****	0.81	*****	0.81	*****	0.81	*****	0.81	*****
14.30	130.	0.40	*****	*****	2.00	*****	0.38	*****	0.14	*****	0.80	*****	80.3	*****	80.3	*****	80.3	*****	80.3	*****	80.3	*****	80.3	*****
14.42	142.	0.40	*****	*****	0.40	*****	0.10	*****	0.24	*****	0.07	*****	0.31	*****	0.31	*****	0.31	*****	0.31	*****	0.31	*****	0.31	*****
14.45	145.	0.40	*****	*****	1.50	*****	0.69	*****	0.06	*****	0.04	*****	0.21	*****	0.21	*****	0.21	*****	0.21	*****	0.21	*****	0.21	*****
15.00	160.	0.40	*****	*****	0.40	*****	0.10	*****	0.24	*****	0.09	*****	0.31	*****	0.31	*****	0.31	*****	0.31	*****	0.31	*****	0.31	*****
15.14	174.	0.40	*****	*****	1.00	*****	0.62	*****	0.07	*****	0.13	*****	0.30	*****	0.30	*****	0.30	*****	0.30	*****	0.30	*****	0.30	*****
15.30	190.	0.40	*****	*****	0.30	*****	0.10	*****	0.15	*****	0.10	*****	0.87	*****	0.87	*****	0.87	*****	0.87	*****	0.87	*****	0.87	*****
15.44	204.	0.30	*****	*****	0.60	*****	0.55	*****	0.07	*****	0.28	*****	78.5	*****	78.5	*****	78.5	*****	78.5	*****	78.5	*****	78.5	*****
16.00	220.	0.30	*****	*****	0.30	*****	0.10	*****	0.29	*****	0.18	*****	1.33	*****	1.33	*****	1.33	*****	1.33	*****	1.33	*****	1.33	*****
16.13	233.	0.30	*****	*****	0.40	*****	0.40	*****	0.93	*****	0.20	*****	74.9	*****	74.9	*****	74.9	*****	74.9	*****	74.9	*****	74.9	*****
16.15	235.	0.30	*****	*****	0.30	*****	0.10	*****	0.57	*****	0.22	*****	1.49	*****	1.49	*****	1.49	*****	1.49	*****	1.49	*****	1.49	*****
16.32	252.	0.40	*****	*****	0.40	*****	0.10	*****	0.57	*****	0.57	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
16.45	265.	0.40	*****	*****	0.40	*****	0.40	*****	0.57	*****	0.57	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
17.00	280.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****

BAG-202  
SURROGATE CONTROL #2  
1979 OCT 25

TIME (POT)  
0913-1048 BAG#11 FILLED WITH PURE AIR FROM CHAMBER SYSTEM  
BAG VOLUME APPROXIMATELY 32 CUBIC METERS  
0920 BAG COVERED  
1121 RH=30% AT T=30 DEG C  
1123 2.6 ML NO2 INJECTED AND MIXED  
1125 7.3 ML NO INJECTED AND MIXED  
1132 14.0 ML N-BUTANE INJECTED  
1132 4.9 ML PROPYLENE INJECTED AND MIXED  
1155 BAG MIXED THOROUGHLY AND DIVIDED FAIR LET OUT TO DIVIDE BAG  
1217 BAG UNCOVERED  
1650 SIDE 2 PARTIALLY SHADED

\*MEASUREMENTS SO MARKED INCLUDE THE FOLLOWING UNITS AND FACTORS:  
R-SCAT (METERS-1) X F+4  
CONDENSATION NUCLEI (PART/CUBIC CM) X E-3  
AEROSOL NUMBER (PART/CUBIC CM) X E-3  
AEROSOL SURFACE (U-METERS2/CUBIC CM) X E-2  
AEROSOL VOLUME (CUBIC U-METERS/CUBIC CM) X 1  
UV (CAL/CM2-MIN) X 1

T=0 AT 1217 PST

TS DEG K AVERAGE 300.7  
UV AVERAGE 0.003

\* ASSIGNED INITIAL CONDITION

BAG-202  
SURROGATE CONTRL #2  
1979 OCT 25

CLOCK	ELAPSED TIME (MIN)	OZONE PPM	OZONE PPM	OZONE PPM	OZONE PPM	NO PPM	NO PPM	NO2-CORR PPM	NO2-CORR PPM	NOX-CORR PPM	NOX-CORR PPM
		SIDE 1	SIDE 2	SIDE 1	SIDE 2	SIDE 1	SIDE 2	SIDE 1	SIDE 2	SIDE 1	SIDE 2
1100	-77.	***	***	***	***	***	***	***	***	***	***
1101	-76.	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1115	-62.	***	***	***	***	***	***	***	***	***	***
1141	-35.	0.003	0.002	0.002	0.002	0.141	0.141	0.071	0.071	0.205	0.205
1145	-32.	***	***	***	***	***	***	***	***	***	***
1158	-19.	0.063	0.003	0.003	0.003	0.141	0.141	0.070	0.070	0.203	0.203
1206	-11.	***	***	***	***	0.004	0.004	0.139	0.139	0.200	0.200
1230	13.	0.004	0.009	0.009	0.009	0.131	0.131	0.079	0.079	0.206	0.206
1242	25.	***	***	***	***	0.012	0.012	0.122	0.122	0.203	0.203
1300	43.	0.005	0.013	0.013	0.013	0.118	0.118	0.091	0.091	0.200	0.200
1313	56.	***	***	***	***	0.015	0.015	0.107	0.107	0.199	0.199
1330	73.	0.014	0.016	0.016	0.016	0.098	0.098	0.102	0.102	0.197	0.197
1341	84.	***	***	***	***	0.018	0.018	0.092	0.092	0.195	0.195
1400	103.	0.015	0.016	0.016	0.016	0.083	0.083	0.121	0.121	0.196	0.196
1415	118.	***	***	***	***	0.019	0.019	0.078	0.078	0.120	0.120
1430	133.	0.013	0.017	0.017	0.017	0.074	0.074	0.124	0.124	0.191	0.191
1442	145.	***	***	***	***	0.019	0.019	0.069	0.069	0.131	0.131
1500	163.	0.017	0.018	0.018	0.018	0.064	0.064	0.131	0.131	0.190	0.190
1510	173.	***	***	***	***	0.019	0.019	0.059	0.059	0.121	0.121
1530	193.	0.012	0.017	0.017	0.017	0.057	0.057	0.078	0.078	0.191	0.191
1538	201.	***	***	***	***	0.018	0.018	0.052	0.052	0.145	0.145
1600	223.	0.020	0.023	0.023	0.023	0.050	0.050	0.147	0.147	0.189	0.189
1611	234.	***	***	***	***	0.017	0.017	0.046	0.046	0.150	0.150
1630	253.	0.023	0.013	0.013	0.013	0.047	0.047	0.155	0.155	0.192	0.192
1638	261.	***	***	***	***	0.015	0.015	0.040	0.040	0.152	0.152
1700	283.	0.013	0.010	0.010	0.010	0.039	0.039	0.155	0.155	0.188	0.188
1710	293.	***	***	***	***	0.011	0.011	0.033	0.033	0.159	0.159

BAG-202  
SURROGATE CONTROL #2  
1979 OCT 25

CLOCK	ELAPSED	PAN	PAN	ACETONE	ACETONE	METHANE	METHANE	ETHANE	ETHANE	ETHENE	ETHENE
TIME	T(MIN)	PPM	PPM	PPM	PPM	PPM	PPM	PPM	PPM	PPM	PPM
	SIDE 1	SIDE 2	SIDE 1	SIDE 2	SIDE 1	SIDE 2	SIDE 1	SIDE 2	SIDE 1	SIDE 2	SIDE 1
11:00	-77.	*****	*****	0.0012	0.0012	1.72	1.72	*****	*****	*****	*****
11:01	-76.	0.0	*****	*****	*****	*****	*****	*****	*****	*****	*****
11:15	-62.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
11:41	-36.	0.0	*****	*****	*****	*****	*****	*****	*****	*****	*****
11:45	-32.	*****	*****	0.0016	0.0016	1.68	1.68	0.0076	0.0076	0.0002	0.0047
11:58	-19.	0.0	*****	*****	*****	*****	*****	*****	*****	*****	*****
12:06	-11.	*****	0.0	*****	*****	*****	*****	0.0080	0.0080	0.0044	0.0044
12:30	11.	0.0	*****	*****	*****	*****	*****	*****	*****	*****	*****
12:42	25.	*****	0.0	*****	*****	*****	*****	*****	*****	*****	*****
13:00	43.	0.0	*****	*****	*****	*****	*****	*****	*****	*****	*****
13:13	56.	*****	0.0	*****	*****	*****	*****	*****	*****	*****	*****
13:30	73.	0.001	*****	*****	*****	*****	*****	*****	*****	*****	*****
13:41	84.	*****	0.001	*****	*****	*****	*****	*****	*****	*****	*****
14:00	103.	0.0	*****	*****	*****	*****	*****	*****	*****	*****	*****
14:15	118.	*****	0.001	*****	*****	*****	*****	*****	*****	*****	*****
14:30	133.	0.001	*****	*****	*****	*****	*****	*****	*****	*****	*****
14:42	145.	*****	0.0	*****	*****	*****	*****	*****	*****	*****	*****
15:00	163.	0.001	*****	*****	*****	*****	*****	*****	*****	*****	*****
15:10	173.	*****	0.0	*****	*****	*****	*****	*****	*****	*****	*****
15:30	193.	0.001	*****	*****	*****	*****	*****	*****	*****	*****	*****
15:38	201.	*****	0.0	*****	*****	*****	*****	*****	*****	*****	*****
16:00	223.	0.0	*****	*****	*****	*****	*****	*****	*****	*****	*****
16:11	234.	*****	0.001	*****	*****	*****	*****	*****	*****	*****	*****
16:30	253.	0.0	*****	0.0012	0.0012	1.69	1.69	0.0087	0.0087	0.0042	0.0042
16:38	261.	*****	0.0	*****	*****	*****	*****	*****	*****	*****	*****
17:00	263.	0.001	*****	*****	0.0013	*****	1.69	1.69	0.0081	0.0081	*****
17:10	293.	*****	0.001	*****	*****	*****	*****	*****	*****	*****	*****

BAG-202  
SURROGATE CONTROL #2  
1379 OCT 25

TIME T (MIN)	CLOCK ELAPSED		ACETYLEN		ACETYLEN		ACETYLEN		PROPANE		PROPENE		I-C4		N-C4	
	PPM	PPM	PPM	PPM	PPM	PPM	PPM	PPM	PPM	PPM	PPM	PPM	SIDE 1	SIDE 2	SIDE 1	SIDE 2
1100	-71.	*****	PN-1	PN-2	DMS-1	DMS-2	SIDE 1	SIDE 2	0.0010	0.0239	0.001	0.0015	0.001	0.001	0.001	0.001
1101	-70.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1115	-62.	0.0167	0.0182	0.0182	0.0182	0.0182	0.0182	0.0182	0.0182	0.0182	0.0182	0.0182	0.0182	0.0182	0.0182	0.0182
1141	-36.	0.0111	0.0107	0.0107	0.0107	0.0107	0.0107	0.0107	0.0107	0.0107	0.0107	0.0107	0.0107	0.0107	0.0107	0.0107
1145	-32.	0.0111	0.0107	0.0107	0.0107	0.0107	0.0107	0.0107	0.0107	0.0107	0.0107	0.0107	0.0107	0.0107	0.0107	0.0107
1150	-19.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1206	-11.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1230	13.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1242	25.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1300	43.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1313	56.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1330	73.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1341	84.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1400	103.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1415	118.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1419	133.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1442	145.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1500	163.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1510	173.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1530	193.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1538	201.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1600	223.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1611	234.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1630	253.	0.0121	*****	*****	*****	*****	*****	*****	0.0129	*****	0.0249	*****	0.086	*****	0.356	*****
1639	261.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1700	283.	*****	*****	*****	*****	*****	*****	*****	0.0104	*****	0.0146	*****	0.080	*****	0.346	*****
1710	293.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****

BAG-202  
SURROGATE CONTROL #2  
1979 OCT 25

CLOCK	ELAPSED TIME	TIME (MIN)	1-C4=	1-C4=	1-C4=	1-C5	1-C5	N-C5
			PPM	PPM	PPM	PPM	PPM	PPM
			SIDE 1	SIDE 2	SIDE 1	SIDE 2	SIDE 1	SIDE 2
1100	-77.	0.0002	0.0002	0.0003	0.0003	0.0009	0.0009	0.0005
1101	-76.	***	***	***	***	***	***	***
1115	-62.	***	***	***	***	***	***	***
1141	-36.	***	***	***	***	***	***	***
1145	-32.	***	***	***	***	***	***	***
1158	-19.	***	***	***	***	***	***	***
1206	-11.	***	***	***	***	***	***	***
1230	13.	***	***	***	***	***	***	***
1242	25.	***	***	***	***	***	***	***
1300	43.	***	***	***	***	***	***	***
1313	56.	***	***	***	***	***	***	***
1330	73.	***	***	***	***	***	***	***
1341	84.	***	***	***	***	***	***	***
1400	103.	***	***	***	***	***	***	***
1415	118.	***	***	***	***	***	***	***
1430	133.	***	***	***	***	***	***	***
1442	145.	***	***	***	***	***	***	***
1500	163.	***	***	***	***	***	***	***
1510	173.	***	***	***	***	***	***	***
1530	193.	***	***	***	***	***	***	***
1538	201.	***	***	***	***	***	***	***
1600	223.	***	***	***	***	***	***	***
1611	234.	***	***	***	***	***	***	***
1630	253.	***	***	***	***	***	***	***
1638	261.	***	***	***	***	***	***	***
1700	283.	***	***	***	***	***	***	***
1710	293.	***	***	***	***	***	***	***

BAG-202  
SURROGATE CCNTRCL #2  
1979 OCT 25

CLOCK TIME (MIN)	ELAPSED TIME (MIN)	B-SCAT	B-SCAT	CONDENS.	CONDENS.	AEROSL N	AEROSL N	AEROSL S	AEROSL S	AEROSL V	AEROSL V	TS		TS	
												SIDE 1*	SIDE 2*	SIDE 1*	SIDE 2*
11.00	-17.	***	***	***	***	***	***	***	***	***	***	***	***	***	***
11.01	-16.	0.50	0.50	0.30	0.30	0.28	0.28	0.28	0.28	0.28	0.28	0.5	0.5	0.5	0.5
11.15	-62.	***	***	***	***	***	***	***	***	***	***	***	***	***	***
11.41	-36.	0.50	0.50	0.60	0.60	0.33	0.33	0.33	0.33	0.33	0.33	85.7	85.7	85.7	85.7
11.45	-32.	***	***	***	***	***	***	***	***	***	***	***	***	***	***
11.58	-19.	0.60	0.60	0.40	0.40	0.47	0.47	0.47	0.47	0.47	0.47	0.0035	0.0035	0.0035	0.0035
12.06	-11.	***	***	0.70	0.70	0.80	0.80	0.80	0.80	0.80	0.80	2.95	2.95	2.95	2.95
12.10	13.	0.60	0.60	0.60	0.60	0.48	0.48	0.48	0.48	0.48	0.48	74.9	74.9	74.9	74.9
12.42	25.	***	***	0.70	0.70	0.50	0.50	0.50	0.50	0.50	0.50	3.34	3.34	3.34	3.34
13.00	43.	0.60	0.60	0.30	0.30	0.29	0.29	0.29	0.29	0.29	0.29	0.0037	0.0037	0.0037	0.0037
13.13	56.	***	***	0.60	0.60	0.90	0.90	0.90	0.90	0.90	0.90	0.3	0.3	0.3	0.3
13.30	73.	0.50	0.50	0.10	0.10	0.36	0.36	0.36	0.36	0.36	0.36	0.0043	0.0043	0.0043	0.0043
13.41	84.	***	***	0.70	0.70	1.70	1.70	1.70	1.70	1.70	1.70	0.75	0.75	0.75	0.75
14.00	105.	0.60	0.60	0.10	0.10	0.32	0.32	0.32	0.32	0.32	0.32	0.0035	0.0035	0.0035	0.0035
14.15	119.	***	***	0.70	0.70	2.90	2.90	2.90	2.90	2.90	2.90	0.89	0.89	0.89	0.89
14.30	133.	0.60	0.60	0.20	0.20	0.48	0.48	0.48	0.48	0.48	0.48	0.3	0.3	0.3	0.3
14.42	145.	***	***	0.60	0.60	0.20	0.20	0.20	0.20	0.20	0.20	0.27	0.27	0.27	0.27
15.00	161.	***	***	0.60	0.60	0.37	0.37	0.37	0.37	0.37	0.37	0.0035	0.0035	0.0035	0.0035
15.10	173.	***	***	0.80	0.80	1.40	1.40	1.40	1.40	1.40	1.40	0.75	0.75	0.75	0.75
15.30	193.	0.70	0.70	0.40	0.40	0.60	0.60	0.60	0.60	0.60	0.60	0.0027	0.0027	0.0027	0.0027
15.38	201.	***	***	0.70	0.70	2.20	2.20	2.20	2.20	2.20	2.20	0.2	0.2	0.2	0.2
16.00	223.	***	***	1.00	1.00	0.0	0.0	0.0	0.0	0.0	0.0	0.0020	0.0020	0.0020	0.0020
16.11	234.	0.50	0.50	2.70	2.70	2.37	2.37	2.37	2.37	2.37	2.37	0.2	0.2	0.2	0.2
16.30	253.	***	***	0.80	0.80	0.46	0.46	0.46	0.46	0.46	0.46	0.0025	0.0025	0.0025	0.0025
16.38	261.	***	***	0.60	0.60	2.30	2.30	2.30	2.30	2.30	2.30	76.7	76.7	76.7	76.7
17.00	283.	***	***	1.10	1.10	0.48	0.48	0.48	0.48	0.48	0.48	0.0014	0.0014	0.0014	0.0014
17.10	293.	***	***	0.50	0.50	2.20	2.20	2.20	2.20	2.20	2.20	69.5	69.5	69.5	69.5

BAG-203  
SURROGATE CONTROL #3  
1979 NOV 2

0630-0800 BAG #11 FILLED WITH PURE AIR FROM CHAMBER SYSTEM  
BAG VOLUME APPROXIMATELY 33 CUBIC METERS

- 0845 BAG COVERED  
0847 RH IS 20% AT 19 DEG C  
0904 2.6 ML NO<sub>2</sub> INJECTED AND MIXED  
0906 7.3 ML NO<sub>2</sub> INJECTED AND MIXED  
0911 500 ML SURROGATE J INJECTED AND MIXED  
0915 14.0 MICROLITERS (U-L) 2, 3-DMB, 1.9 U-L TOLUENE,  
1.6 U-L 2-ME-2-C<sub>4</sub>=, AND 5.4 U-L M-XYLENE INJECTED AND MIXED  
0920 BAG DIVIDED  
1012 BAG UNCOVERED  
NO<sub>2</sub> AND NO<sub>x</sub> WERE NOT CORRECTED FOR PAN DUE TO INSTRUMENT  
MALFUNCTION DURING MOST OF EXPERIMENT. MAXIMUM OF 6 PPB  
OBSERVED AT END OF EXPERIMENT.  
1245 TSI WHITBY OBSERVED TO BE DISCONNECTED FROM SAMPLING LINE.  
SOME READINGS FROM OTHER INSTRUMENTS MAY BE AFFECTED  
SIDE 1 AND SIDE 2 POSSIBLY RECEIVING DIFFERENT AMOUNTS OF SUNLIGHT  
DASIBI 1770 AND BENIX O<sub>3</sub> ANALYZERS, TSI 3030 (WHITBY).  
CLIMET OPTICAL COUNTER USED

\*MEASUREMENTS SO MARKED INCLUDE THE FOLLOWING UNITS AND FACTORS:

B-SCAT	(METERS-1)	X E+4
CONDENSATION NUCLEI	(PART/CUBIC CM)	X E-3
AEROSOL NUMBER	(PART/CUBIC CM)	X E-3
AEROSOL SURFACE	(U-METERS <sup>2</sup> /CUBIC CM)	X E-2
AEROSOL VOLUME	(CUBIC U-METERS/CUBIC CM)	X 1
UV	(CAL/CM <sup>2</sup> -MIN)	X 1

T=0 AT 1012 PST

TS DEG K AVERAGE  
UV AVERAGE

301.5  
0.004  
\* ASSIGNED INITIAL CONDITION

3AG-203 SURROGATE CONTROL #2  
1979 NJV 2

BLOCK	ELAPSED TIME (MIN)	OZONE PPM	OZONE PPM	OZONE PPM	OZONE PPM	NO PPM	NOX-CORR PPM	NOX-CURR PPM	NOX-CURR PPM	NOX-CORR PPM							
829	-103.	0.005	*****	0.005	*****	0.001	*****	0.001	*****	0.009	*****	0.010	*****	0.010	*****	0.010	*****
930	-42.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
932	-40.	0.02B	*****	0.003	*****	0.159	*****	0.153	*****	0.084	*****	0.235	*****	0.235	*****	0.235	*****
941	-31.	*****	0.005	*****	0.003	0.003	*****	0.153	*****	0.081	*****	0.228	*****	0.228	*****	0.228	*****
1005	-7.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1015	3.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1016	4.	0.007	*****	0.009	*****	0.159	*****	0.159	*****	0.082	*****	0.233	*****	0.233	*****	0.233	*****
1023	11.	*****	0.004	*****	0.010	*****	0.145	*****	0.087	*****	0.087	*****	0.221	*****	0.221	*****	0.221
1045	33.	0.010	*****	0.013	*****	0.129	*****	0.129	*****	0.107	*****	0.225	*****	0.225	*****	0.225	*****
1051	39.	*****	0.011	*****	0.013	*****	0.119	*****	0.119	*****	0.108	*****	0.216	*****	0.216	*****	0.216
1100	48.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1115	63.	0.033	*****	0.017	*****	0.092	*****	0.139	*****	0.132	*****	0.223	*****	0.223	*****	0.223	*****
1122	70.	*****	0.028	*****	0.019	*****	0.086	*****	0.086	*****	0.159	*****	0.213	*****	0.213	*****	0.213
1145	93.	0.031	*****	0.028	*****	0.064	*****	0.064	*****	0.107	*****	0.200	*****	0.200	*****	0.200	*****
1152	100.	*****	0.034	*****	0.029	*****	0.061	*****	0.061	*****	0.150	*****	0.195	*****	0.195	*****	0.195
1215	123.	*****	0.040	*****	0.038	*****	0.043	*****	0.043	*****	0.165	*****	0.197	*****	0.197	*****	0.197
1221	129.	0.045	*****	0.045	*****	0.039	*****	0.039	*****	0.175	*****	0.199	*****	0.199	*****	0.199	*****
1230	138.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1245	153.	0.064	*****	0.065	*****	0.031	*****	0.031	*****	0.188	*****	0.204	*****	0.204	*****	0.204	*****
1249	157.	*****	0.055	*****	0.059	*****	0.028	*****	0.028	*****	0.171	*****	0.191	*****	0.191	*****	0.191
1315	183.	0.036	*****	0.084	*****	0.021	*****	0.021	*****	0.189	*****	0.197	*****	0.197	*****	0.197	*****
1322	190.	*****	0.068	*****	0.078	*****	0.019	*****	0.019	*****	0.171	*****	0.191	*****	0.191	*****	0.191
1345	213.	0.101	*****	0.103	*****	0.017	*****	0.017	*****	0.183	*****	0.188	*****	0.188	*****	0.188	*****
1352	220.	*****	0.030	*****	0.086	*****	0.017	*****	0.017	*****	0.173	*****	0.178	*****	0.178	*****	0.178
1400	228.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1415	243.	0.106	*****	0.120	*****	0.012	*****	0.012	*****	0.185	*****	0.190	*****	0.190	*****	0.190	*****
1422	250.	*****	0.095	*****	0.099	*****	0.010	*****	0.010	*****	0.171	*****	0.171	*****	0.171	*****	0.171
1445	273.	0.115	*****	0.132	*****	0.009	*****	0.009	*****	0.180	*****	0.174	*****	0.174	*****	0.174	*****
1455	283.	*****	0.098	*****	0.109	*****	0.005	*****	0.005	*****	0.171	*****	0.167	*****	0.167	*****	0.167
1516	304.	0.120	*****	0.130	*****	0.004	*****	0.004	*****	0.179	*****	0.173	*****	0.173	*****	0.173	*****
1525	313.	*****	0.094	*****	0.119	*****	0.002	*****	0.002	*****	0.170	*****	0.165	*****	0.165	*****	0.165
1530	318.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****

BAG-203  
SURRGATE CONTROL #3  
1979 NW 2

CLOCK TIME ELAPSED TIME (MIN)	PAN PPM	ACETONE PPM	MEK PPM	METHANE PPM	ETHANE PPM	ETHENE PPM	SIDE 1		SIDE 2	
							SIDE 1 STD 1	SIDE 2 STD 2	SIDE 1 STD 1	SIDE 2 STD 2
829 -103.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
930 -42.	*****	*****	*****	*****	0.0040	*****	*****	*****	*****	*****
932 -40.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
941 -31.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1005 -7.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1015 3.	*****	*****	*****	*****	0.0065	*****	*****	*****	*****	*****
1016 4.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1023 11.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1045 33.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1051 39.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1100 48.	*****	*****	*****	*****	0.0110	*****	*****	*****	*****	*****
1115 63.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1122 70.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1145 93.	*****	*****	*****	*****	0.0170	*****	*****	*****	*****	*****
1152 100.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1215 123.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1221 129.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1230 138.	*****	*****	*****	*****	0.0179	*****	*****	*****	*****	*****
1245 153.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1249 157.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1315 183.	*****	*****	*****	*****	0.0233	*****	*****	*****	*****	*****
1322 190.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1345 213.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1352 220.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1400 228.	*****	*****	*****	*****	0.0247	*****	*****	*****	*****	*****
1415 243.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1422 250.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1445 273.	*****	*****	*****	*****	0.0267	*****	*****	*****	*****	*****
1455 283.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1516 304.	*****	*****	*****	*****	0.0202	*****	*****	*****	*****	*****
1525 313.	*****	*****	*****	*****	0.0262	*****	*****	*****	*****	*****
1530 318.	*****	*****	*****	*****	0.0266	*****	*****	*****	*****	*****
						0.0060	*****	*****	1.19	*****
							*****	*****	0.0672	*****
										0.0314

BAG-203  
SURROGATE CONTRACT #2  
1977 NJV 2

CLOCK TIME	ELAPSED TIME	ACETYLEN		PROPYANE		PROPENE		1-C4		N-C4	
		PPM	PPM	PPM	PPM	PPM	PPM	PPM	PPM	PPM	PPM
829	-103.	* * * * *	* * * * *	DMS-1	SIDE 1	* * * * *	* * * * *	* * * * *	* * * * *	SIDE 1	SIDE 2
930	-42.	* * * * *	* * * * *	DMS-2	SIDE 2	* * * * *	* * * * *	* * * * *	* * * * *	SIDE 1	SIDE 2
932	-40.	* * * * *	* * * * *	0.0496	0.0486	0.0337	0.0337	0.012	0.012	0.0011	0.0011
941	-31.	* * * * *	* * * * *	0.0384	0.0384	0.0477	0.0477	0.012	0.012	0.0012	0.0012
1005	-7.	* * * * *	* * * * *	0.0406	0.0406	0.0319	0.0319	0.010	0.010	0.0011	0.0011
1015	3.	* * * * *	* * * * *	0.0399	0.0399	0.0452	0.0452	0.010	0.010	0.0011	0.0011
1016	4.	* * * * *	* * * * *	0.0418	0.0418	0.0473	0.0473	0.008	0.008	0.0011	0.0011
1023	11.	* * * * *	* * * * *	0.0419	0.0419	0.0329	0.0329	0.008	0.008	0.0011	0.0011
1045	33.	* * * * *	* * * * *	0.0420	0.0420	0.0319	0.0319	0.010	0.010	0.0011	0.0011
1051	39.	* * * * *	* * * * *	0.0421	0.0421	0.0319	0.0319	0.010	0.010	0.0011	0.0011
1100	43.	* * * * *	* * * * *	0.0422	0.0422	0.0319	0.0319	0.010	0.010	0.0011	0.0011
1115	63.	* * * * *	* * * * *	0.0423	0.0423	0.0319	0.0319	0.010	0.010	0.0011	0.0011
1122	70.	* * * * *	* * * * *	0.0424	0.0424	0.0319	0.0319	0.010	0.010	0.0011	0.0011
1145	93.	* * * * *	* * * * *	0.0425	0.0425	0.0319	0.0319	0.010	0.010	0.0011	0.0011
1152	100.	* * * * *	* * * * *	0.0426	0.0426	0.0319	0.0319	0.010	0.010	0.0011	0.0011
1215	123.	* * * * *	* * * * *	0.0427	0.0427	0.0319	0.0319	0.010	0.010	0.0011	0.0011
1221	129.	* * * * *	* * * * *	0.0428	0.0428	0.0319	0.0319	0.010	0.010	0.0011	0.0011
1230	139.	* * * * *	* * * * *	0.0429	0.0429	0.0319	0.0319	0.010	0.010	0.0011	0.0011
1245	151.	* * * * *	* * * * *	0.0430	0.0430	0.0319	0.0319	0.010	0.010	0.0011	0.0011
1249	157.	* * * * *	* * * * *	0.0431	0.0431	0.0319	0.0319	0.010	0.010	0.0011	0.0011
1315	183.	* * * * *	* * * * *	0.0432	0.0432	0.0319	0.0319	0.010	0.010	0.0011	0.0011
1322	190.	* * * * *	* * * * *	0.0433	0.0433	0.0319	0.0319	0.010	0.010	0.0011	0.0011
1345	213.	* * * * *	* * * * *	0.0434	0.0434	0.0319	0.0319	0.010	0.010	0.0011	0.0011
1352	220.	* * * * *	* * * * *	0.0435	0.0435	0.0319	0.0319	0.010	0.010	0.0011	0.0011
1400	224.	* * * * *	* * * * *	0.0436	0.0436	0.0319	0.0319	0.010	0.010	0.0011	0.0011
1415	243.	* * * * *	* * * * *	0.0437	0.0437	0.0319	0.0319	0.010	0.010	0.0011	0.0011
1422	250.	* * * * *	* * * * *	0.0438	0.0438	0.0319	0.0319	0.010	0.010	0.0011	0.0011
1445	273.	* * * * *	* * * * *	0.0439	0.0439	0.0319	0.0319	0.010	0.010	0.0011	0.0011
1455	283.	* * * * *	* * * * *	0.0440	0.0440	0.0319	0.0319	0.010	0.010	0.0011	0.0011
1516	304.	* * * * *	* * * * *	0.0441	0.0441	0.0319	0.0319	0.010	0.010	0.0011	0.0011
1525	313.	* * * * *	* * * * *	0.0442	0.0442	0.0319	0.0319	0.010	0.010	0.0011	0.0011
1530	314.	* * * * *	* * * * *	0.0443	0.0443	0.0319	0.0319	0.010	0.010	0.0011	0.0011

BAG-203  
SURROGATE CONTROL #3  
1979 NOV 2

CLOCK TIME	ELAPSED TIME	1-C4=		I-C4=		T2-C4=		I-C5=		CIS2-C4=		N-C5=	
		PPM	SIDE 1	PPM	SIDE 2	PPM	SIDE 1	PPM	SIDE 2	PPM	SIDE 1	PPM	SIDE 2
829	-103.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
930	-42.	0.0001	0.0001	0.0002	0.0002	0.0007	0.0007	0.0005	0.0155	0.0155	0.0018	0.0018	0.0018
932	-4.0.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
941	-31.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1005	-7.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1915	3.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1916	4.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1023	11.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1045	33.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1951	39.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1100	4.8.	*****	*****	0.0002	*****	0.0001	*****	0.0003	*****	0.0005	*****	0.0007	*****
1115	6.3.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1122	70.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1145	93.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1152	100.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1215	123.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1221	129.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1230	138.	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0006	0.0023	0.0023	0.0002	0.0002	0.0002
1245	153.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1249	157.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1315	183.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1322	190.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1345	213.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1352	220.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1400	228.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1415	243.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1422	250.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1445	273.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1455	283.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1516	304.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1525	313.	*****	*****	0.0002	*****	0.0001	*****	0.0007	*****	0.0001	*****	0.0003	0.0003
1530	318.	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****

BAG-203  
SURRGATE CONTROL #3  
1979 NOV 2

CLOCK	ELAPSED	2ME-C4=2	2ME-C4=2	2,3-DMS	2,3-DMS	TOLUENE	TOLUENE	M-XYL	M-XYL
TIME	MIN	PPM	PPM	PPM	PPM	PPM	PPM	PPM	PPM
		SIDE 1	SIDE 2	SIDE 1	SIDE 2	SIDE 1	SIDE 2	SIDE 1	SIDE 2
829.	-103.	*****	*****	*****	*****	*****	*****	*****	*****
930.	-42.	0.0115	0.0115	0.0022	0.0322	0.014	0.014	0.0353	0.0353
932.	-40.	*****	*****	*****	*****	*****	*****	*****	*****
941.	-31.	*****	*****	*****	*****	*****	*****	*****	*****
1005.	-7.	*****	*****	*****	*****	*****	*****	*****	*****
1015.	3.	0.0076	0.0076	0.0015	0.0015	0.014	0.014	0.0350	0.0350
1016.	4.	*****	*****	*****	*****	*****	*****	*****	*****
1023.	11.	*****	*****	*****	*****	*****	*****	*****	*****
1045.	33.	*****	*****	*****	*****	*****	*****	*****	*****
1051.	39.	*****	*****	*****	*****	*****	*****	*****	*****
1100.	48.	*****	*****	0.0016	0.0016	0.013	0.013	0.0290	0.0290
1115.	63.	*****	*****	*****	*****	*****	*****	*****	*****
1122.	70.	*****	*****	*****	*****	*****	*****	*****	*****
1145.	93.	0.0014	0.0014	0.0747	0.0747	0.013	0.013	0.0256	0.0256
1152.	100.	*****	*****	*****	*****	*****	*****	*****	*****
1215.	123.	*****	*****	*****	*****	*****	*****	*****	*****
1221.	129.	*****	*****	*****	*****	*****	*****	*****	*****
1230.	130.	0.0002	0.0002	0.0031	0.0031	0.012	0.012	0.0211	0.0211
1245.	153.	*****	*****	*****	*****	*****	*****	*****	*****
1249.	157.	*****	*****	*****	*****	*****	*****	*****	*****
1315.	193.	*****	*****	0.0686	0.0686	0.012	0.012	0.0193	0.0193
1322.	190.	*****	*****	*****	*****	*****	*****	*****	*****
1345.	213.	*****	*****	*****	*****	*****	*****	*****	*****
1352.	223.	*****	*****	*****	*****	*****	*****	*****	*****
1400.	228.	*****	*****	0.0002	0.0629	0.011	0.011	0.0169	0.0169
1415.	243.	*****	*****	*****	*****	*****	*****	*****	*****
1422.	250.	*****	*****	*****	*****	*****	*****	*****	*****
1445.	273.	0.0001	0.0001	0.0658	0.0658	0.011	0.011	0.0161	0.0161
1455.	283.	*****	*****	*****	*****	*****	*****	*****	*****
1516.	304.	*****	*****	*****	*****	*****	*****	*****	*****
1525.	313.	*****	*****	*****	*****	*****	*****	*****	*****
1530.	318.	*****	0.0	0.0614	0.0614	0.011	0.011	0.0149	0.0149

BAG-203  
SURROGATE CONTROL #3  
1979 NJV 2

CLOCK	ELAPSED TIME (MIN)	B-SCAT	CONDENS.	CONDENS.	AEROSL N	AEROSL S	AEROSL V	TS	DEG F	DEG F	TS
029	-103.	0.40	*****	*****	0.0	*****	0.0	*****	0.0	*****	65.9
330	-42.	0.40	*****	*****	0.0	*****	0.0	*****	0.0	*****	65.9
932	-40.	0.40	*****	*****	0.0	*****	0.0	*****	0.0	*****	65.9
941	-31.	0.40	*****	*****	0.0	*****	0.0	*****	0.0	*****	65.9
1005	-7.	0.40	*****	*****	0.0	*****	0.0	*****	0.0	*****	65.9
1015	3.	0.40	*****	*****	0.0	*****	0.0	*****	0.0	*****	65.9
1016	4.	0.30	*****	*****	0.0	*****	0.0	*****	0.0	*****	65.9
1023	11.	0.30	*****	*****	0.0	*****	0.0	*****	0.0	*****	65.9
1045	33.	0.30	*****	*****	0.0	*****	0.0	*****	0.0	*****	65.9
1051	39.	0.30	*****	*****	0.0	*****	0.0	*****	0.0	*****	65.9
1100	48.	0.30	*****	*****	0.0	*****	0.0	*****	0.0	*****	65.9
1115	63.	0.30	*****	*****	0.0	*****	0.0	*****	0.0	*****	62.1
1122	70.	0.30	*****	*****	0.0	*****	0.0	*****	0.0	*****	62.1
1145	93.	0.30	*****	*****	0.0	*****	0.0	*****	0.0	*****	62.1
1152	100.	0.30	*****	*****	0.0	*****	0.0	*****	0.0	*****	62.1
1215	121.	0.30	*****	*****	0.0	*****	0.0	*****	0.0	*****	62.1
1221	129.	0.30	*****	*****	0.0	*****	0.0	*****	0.0	*****	62.1
1230	138.	0.30	*****	*****	0.0	*****	0.0	*****	0.0	*****	62.1
1245	153.	0.30	*****	*****	0.0	*****	0.0	*****	0.0	*****	62.1
1249	157.	0.30	*****	*****	0.0	*****	0.0	*****	0.0	*****	62.1
1315	163.	0.30	*****	*****	0.0	*****	0.0	*****	0.0	*****	62.1
1322	199.	0.30	*****	*****	5.00	*****	2.07	*****	0.29	*****	87.5
1345	213.	0.30	*****	*****	0.10	*****	0.82	*****	0.10	*****	85.7
1352	220.	0.30	*****	*****	4.40	*****	4.40	*****	2.59	*****	85.7
1400	228.	0.30	*****	*****	3.70	*****	3.70	*****	1.55	*****	83.9
1415	243.	0.30	*****	*****	0.70	*****	1.14	*****	0.14	*****	83.9
1422	250.	0.20	*****	*****	0.30	*****	0.60	*****	0.13	*****	83.9
1445	275.	0.30	*****	*****	0.40	*****	1.11	*****	0.20	*****	83.9
1455	283.	0.30	*****	*****	3.90	*****	6.12	*****	0.53	*****	83.9
1516	304.	0.30	*****	*****	0.70	*****	1.11	*****	0.16	*****	80.3
1525	313.	0.30	*****	*****	4.10	*****	3.96	*****	0.44	*****	80.3
1530	318.	0.30	*****	*****	4.44	*****	3.96	*****	0.09	*****	80.3

BAG-203  
SURROGATE CCNTPCL #3  
1979 NW 2

CLOCK TIME	FLAPS C/D	UV	UV	SIDE 1*	SIDE 2*
TIME	T (MIN)				
829	-10.3.	*****	*****	*****	*****
930	-4.2.	*****	*****	*****	*****
932	-4.0.	0.0037	0.0037	*****	*****
941	-3.1.	*****	*****	0.0036	*****
1005	-7.	*****	*****	*****	*****
1015	3.	*****	*****	*****	*****
1016	4.	0.0039	0.0039	*****	*****
1023	1.1.	*****	*****	*****	*****
1045	3.3.	0.0040	0.0040	*****	*****
1051	3.9.	*****	*****	*****	*****
1100	4.8.	*****	*****	*****	*****
1115	6.3.	0.0044	0.0044	*****	*****
1122	7.0.	*****	*****	*****	*****
1145	9.3.	0.0040	0.0040	*****	*****
1152	10.0.	*****	*****	*****	*****
1215	12.3.	*****	*****	0.0036	*****
1221	12.9.	*****	*****	*****	*****
1230	13.8.	*****	*****	*****	*****
1245	15.3.	0.0037	0.0037	*****	*****
1249	15.7.	*****	*****	*****	*****
1315	1d3.	0.0034	0.0034	*****	*****
1322	19.0.	*****	*****	*****	*****
1345	21.3.	0.0036	0.0036	*****	*****
1352	22.0.	*****	*****	*****	*****
1400	22.9.	*****	*****	*****	*****
1415	24.3.	0.0034	0.0034	*****	*****
1422	25.0.	*****	*****	*****	*****
1445	27.3.	0.0020	0.0020	*****	*****
1452	28.3.	*****	*****	*****	*****
1516	30.4.	0.0026	0.0026	*****	*****
1525	31.1.	*****	*****	*****	*****
1530	31.0.	*****	*****	*****	*****